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Theoretical studies of naphthoquinone reactivity toward amines

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THEORETICAL STUDIES OF NAPHTHOQUINONE REACTIVITY TOWARD AMINES

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ABSTRACT

Quinones are a class of organic compounds containing a six-membered unsaturated cyclic ring with two carbonyl groups and are biologically relevant due to their ability to participate in redox reactions. Experiments have showed that quinones can induce protein modifications including oligomerization and polymerization by binding to proteins. To complement these experimental studies, theoretical studies of naphthoquinone reactivity toward an amino group were conducted. The reactions between three naphthoquinones, 1,2-naphthoquinone (ONQ), 1,4-naphthoquinone (PNQ), and 2-hydroxy-1,4-naphthoquinone (HNQ), and methylamine, a N-containing nucleophile, were investigated. For each naphthoquinone, the first step of both 1,2- and 1,4-additions at all possible C=O positions were examined. For ONQ and HNQ, it was found that the 1,2-additions are more likely to occur than the 1,4-additions, while for PNQ, the 1,4-addition is more likely. The computations showed that ONQ is predicted to be the most reactive, followed by HNQ, and lastly PNQ. All theoretical calculations were performed using a hybrid density functional theory method, MPW1K, in conjunction with the 6-31+G(d,p) basis set.

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LIST OF ACRONYMS

C1	Carbonyl 1
C2	Carbonyl 2
C4	Carbonyl 4
CBQ	chloro-1,4-benzoquinone
DFT	Density functional theory
ETC	Electron Transport Chain
HDFT	Hybrid density functional theory
HF	Hartree-Fock
HNQ	2-hydroxy-1,4-naphthoquinone or Hydroxynaphthoquinone
MBQ	methyl-1,4-benzoquinone
MPW1B95	Modified Perdew-Wang exchange functional and Beck's correlation functional method
MPWB1K	Modified Perdew-Wang exchange functional and Beck's correlation functional method
PAH(s)	Polycyclic aromatic hydrocarbons (s)
PhBQ	phenyl-1,4-benzoquinone
PNQ	1,4-naphthoquinone or *para*-naphthoquinone
ONQ	1,2-naphthoquinone or *ortho*-naphthoquinone
SDS-PAGE	Sodium Dodecyl Sulfate Polyacrylamide Gel Electrophoresis
TCBQ	tetrachloro-1,4-benzoquinone
UV-Vis	Ultraviolet-Visible

CHAPTER 1

INTRODUCTION

1.1 Quinones

1.1.1 Brief description of quinones

Quinones are a class of organic compounds containing a six-membered unsaturated cyclic ring with two carbonyl groups that are either adjacent to each other or separated by a double bond. Quinones can be further categorized into three main classes: benzoquinones, naphthoquinones, and anthraquinones where various derivatives exist through the replacement of hydrogen with other groups. Figure 1.1 shows chemical structures of each main type of quinone.

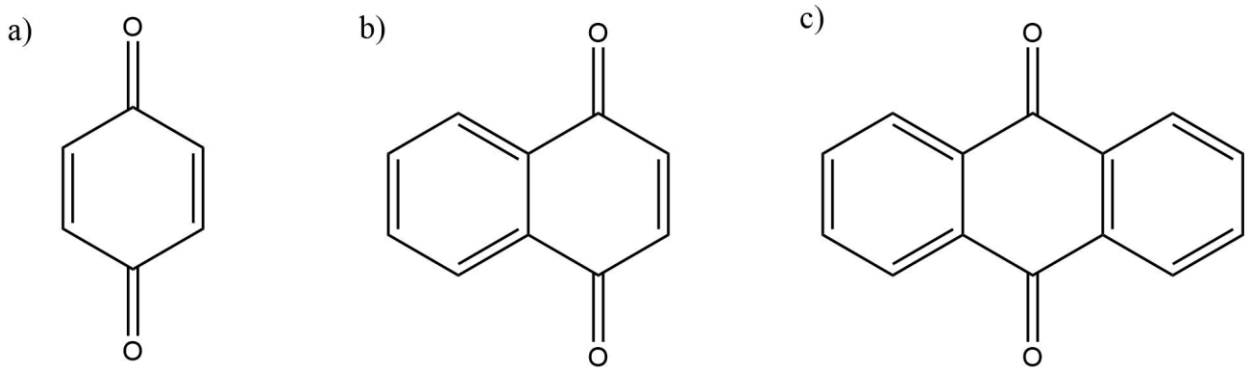


Figure 1.1 Chemical structures of selected quinones
a) 1,4-benzoquinone, b) 1,4-naphthoquinone, c) 9,10-anthraquinone

Quinones are important in various areas from biological processes to industrial production of other chemicals. Naturally, quinones are found in bacteria, certain fungi forms, and various higher plants, and they also exist as biological pigments. In addition, quinones are known to be involved in the redox chemistry of virtually all living organism, as ubiquinone-10 is

involved in the electron transport chain (ETC) in aerobic respiration and plastoquinone is involved in the ETC of photosynthesis [Wass, 2006]. This shows that quinones play an important role in our daily lives.

Some quinones have been recognized for their medicinal value as anticancer, antibacterial, or antimalarial drugs [O'Brian, 1991]. For instance, two natural naphthoquinones, alkannin and shikonin, are known to display wound healing, anti-inflammatory antibacterial, and antitumor properties [Papageorgiou, 1999]. Some other examples of medicinal uses are purgative with sennosdes, anti-microbacterial with rhein- and saprorthoquinone, anti-tumor with emodin and jugone, and anti-cardiovascular disease with tanshinone [Liu, 2011]. These are only some examples of how quinones can be used as treatment for certain diseases. However, there are also quinones that can be toxic to the body.

An interesting class of compounds called polycyclic aromatic hydrocarbons (PAHs) are commonly found in fuels, cigarette smoke, vehicular exhaust, cosmetics, and medicines. With the PAHs in our everyday environment, they can be absorbed into our body and become oxidized to form a group of quinones called polycyclic aromatic hydrocarbon quinones (PAH-quinones) [Muñoz, 2011]. These PAH-quinones can become toxic to the body because they have the ability to perform redox cycling and act as a Michael acceptor [Bolton, 2000]. This allows the PAH-quinones to react with proteins and nucleic acids to change their structure which leads to change of function [Kim et al., 2012; Kim et al., 2015]. There are three ways that quinones can modify proteins: adduct formation, redox cycling, and protein aggregation. Adduct formation occurs when a nitrogen-, sulfur-, or oxygen-containing amino acid on the protein performs a nucleophilic attack on the quinone resulting in the quinone being covalently attached to the protein. In redox cycling, there is a cycling between quinones and their reduced forms that leads

to the formation of reactive oxygen species that can form superoxides. These superoxides can cause oxidative damage to proteins. Lastly, protein aggregation is the process in which quinones react with an amino acid like lysine to oxidize it, and the oxidized lysine is able to join with other lysine residues in other proteins. This leads to cross-linking that make an oligomer, and eventually to protein aggregation [Kim, 2013]. Overall, these different reactions show how dangerous PAH-quinones can be to biological systems since they can change protein structures and alter their function.

1.1.2 Selected experimental studies of quinones

Quinones have been studied for decades and are still an important subject of research for many different fields. This section presents some of the more recent experimental studies conducted on quinones.

One of the most common topics being researched right now is the utilization of the redox potentials of quinones to synthesize other molecules. Qin et al. have studied and reported the use of *ortho*-quinone as a catalyst for the aerobic oxidative dehydrogenation of amines to imines [Qin et al., 2015]. The authors decided to use quinones because mechanistic understanding of how quinone cofactors mediate C–H oxidation of amine. Prior to this research, there have been studies that successfully use quinones in the catalytic oxidative dehydrogenation of linear primary amines to imines and limited success on secondary amine dehydrogenation. The authors looked to develop a quinone-type catalyst that could perform the oxidative dehydrogenation of α-branched amines. Through their studies, Qin et al. identified a simple *ortho*-quinone as a viable catalyst without the use of any metal cocatalyst or additives. To test for the effectiveness of this

quinone, 1-phenylethan-amine was used as a model substrate and a number of quinone-based catalyst were tested. The yields of the products were determined with a ^{1}H NMR analysis. The authors had a breakthrough when the *ortho*-quinone with a methoxyl group showed promising results with high yield compared to the other catalysts. This research is important in its field because it provides researchers a new way to effectively oxidize α-branched primary amines and cyclic secondary amines without the use of metal cocatalysts that could be expensive.

Gurkan et al. studied and reported the redox activity of quinone materials, in the presence of ionic liquids (IL), with the ability to bind reversibly to CO_2 [Gurkan et al., 2015]. Since quinones are redox-active molecules that have significantly higher binding affinity for CO_2 in their reduced form than in their neutral state, the authors wanted to explore the electrocarboxylation of quinones in ionic liquids for potential applications in the separation of CO_2 from gas mixtures. Many different ILs were tested for their suitability as solvents for quinone species by testing for viscosities, quinone solvation capabilities, and electrochemical windows. The quinone that was mainly used in this experiment was 1,4-napthoquinone. Cyclic voltammetry was utilized to measure the hydrogen-bonding affinity between quinones and ILs, and UV-Vis spectroscopy was used to test quinone solubility. The results showed that 1,4-naphthoquinone and 1-ethyl-3-methylimidazolium tricyanomethanide had a higher quinone solubility compared to the other ionic liquids and common solvents. It was shown that this system was able to separate CO_2 from dilute gas mixtures that came in contact with the cathode by overcoming back-diffusive transport of CO_2 from the anodic side. This research is interesting because it opens the possibility of using quinones as material to remove CO_2 from our surroundings. It also formulated a new model for electrochemical separation of CO_2 that can be further studied.

Tu et al. studied and reported on the potential health effects of quinones form natural products like phenols and catechols [Tu et al., 2011]. Many phenols and catechols are known as antioxidants and have putative disease-preventive properties, but there are some that can have negative health effects. One possible explanation for the toxicity examined in this study is the bioactivation of phenolic function to quinones that are capable of modifying DNA and proteins. Tu et al. used mass spectrometry to study four quinones that are produced by oxidizing flavanones and flavones to see their structure toxicity relationship. The results of the experiment showed that quinones containing a C2–C3 single bond have higher aqueous stability and longer half-lives than those with double bonds in the same position. In addition, the quinones with the double bonds at the C2–C3 show little ability to depurinate DNA since it hydrates to an unreactive species. These results support the idea that there is a highly structure-dependent mechanism of quinone hydration at the C2–C3 double bond in the flavonoid structure. For quinones other than those that originate from flavonoids, the authors believe that the structural determinant may be any double bond on a conjugatable position to a quinone function. This might encourage further investigation into chemical structure-property relationships of other biologically important quinones.

These are only some of the experimental studies that are currently being conducted on quinones, and these studies encompass a wide variety of disciplines.

1.1.3 Selected theoretical studies of quinones

Tarumi et al. studied the reaction mechanisms of the Takahax process, the industrial desulfurization process used in Japanese steel-works to remove hydrogen sulfide from coke oven

gas. In this process, H_2S is being oxidized by 1,4-naphthoquinone-2-sulfonic acid (NQS) to become the reduced form, 1,4-dihydroxynaphthalene-2-sulfonic acid. In this reaction, NQS can be regarded as a catalyst. To better understand this reaction, density functional theory calculations were performed using Gaussian 09 where the molecular geometries were optimized at the B3LYP/6-31+G(d) level theory combined with the continuum solvation model based on density (SMD). The authors also adopted a cluster-continuum model where explicit water molecules are incorporated into the framework. Based on their models, the rate-determining step was determined to be the reaction where the first hydrogen atom is transferred. This reaction was characterized as proton-coupled electron transfer because the proton and electron are transferred through different pathways. The results of this study suggest that the catalysts need to be quinone compounds with well-balanced HOMO//LUMO energies, and this might be helpful in the development of new catalyst.

Ambati et al. used density functional theory to study the semiquinone radical anions of polychlorinated biphenyls (PCBs) [Ambati et al., 2012]. Since these radicals are of high reactivity, a computational method was needed to study their role in PCB-induced toxicity and the structure-role relationship. The unrestricted B3LYP/6-311G** method was used to investigate molecular descriptors of the syn-and anti-like conformations of the PCB semiquinone radical anions. The molecular descriptors displayed some dependence on the conformation, especially for *ortho*-substituted PCB semiquinone radical anions. In addition, the anti-like conformation of the *ortho*-substituted PCB semiquinone radical anion was determined to be more stable than the syn-like conformation, and the opposite is true for the parent PCB quinone. This might suggest that the syn- and anti- like conformations of the semiquinone radical anions

can interact differently with target molecules, which may suggest different roles of these conformations in the toxicity of PCBs.

An interesting study was done by Hughes and Swamidass who wanted to find a way to predict quinone species formation in drug metabolism in the body [Hughes and Swamidass, 2017]. By detecting or anticipating quinone formation, one could avoid drug candidates that can form reactive metabolites for drug development. For this study, they decided focus on quinones as an indicator because it they are the most common type of reactive metabolites as over 40% of all known reactive metabolites. Although there are experimental methods for detecting quinone formation, they require time and resources. To create a quick and reliable screening method, they used a deep learning approach to create a method that has a high accuracy in predicting atom pairs and molecules that form quinones that form with quinones. This led to the creation of the QP-trained quinone formation model that was built using a deep convolutional neural network that calculated molecular quinone formation scores, pair quinone formation scores, and atom quinone formation scores. The model was built using their in-house Python software to define atoms and molecules, while quantum chemistry calculations like MOPAC was used in predicting sites of metabolism. After building the backbone of the network, the network was trained to give accurate scores for each type of formation. After testing out the model, it was determined to be a good predictor of quinone formation. This is an interesting study because of how it uses the formation of quinones, an important reactive metabolite in our body, to give us early warning signs to drug metabolism that should not be occurring.

1.1.4 Prior experimental studies on protein modifications by quinones

Over the years, many studies have been conducted in our labs regarding lysozyme, Ribonuclease A, and their interactions with various quinones. These studies are important because they explain why this research is being conducted, and it also gives experimental data to compare our computational results to. In fact, the initial findings were very important because they encouraged further research into other types of quinones.

The first study conducted in our labs was the modification of Ribonuclease A induced by 1,4-benzoquinone or *p*-benzoquinone (PBQ) [Kim et al., 2012]. In one set of experiments presented in this study, the concentration of Ribonuclease A was fixed at 0.050 mM while the concentration of the PBQ was at various concentrations (0.050, 0.25, 0.50, 1.50 mM). The reactions were carried out using a phosphate buffer at pH=7.0 and 37°C. The protein modification was tested and shown using fluorescence, UV-Vis, SDS-PAGE, and confocal microscopy. Fluorescence spectroscopy and UV-Vis spectroscopy were utilized to examine the spectrophotometric characteristics of Ribonuclease A after exposure to PBQ. SDS-PAGE was used to visualize the polymeric aggregates formed by the reactions. The results showed that an increase in the concentration of the PBQ led to an increase in the efficiency of protein modification. In addition, the study also determined that PBQ does elicit modification of Ribonuclease A by forming both Ribonuclease adducts and polymeric aggregates.

Following the original study, another study focusing on the comparison of Ribonuclease A modifications induced by substituted PBQs directly builds on the findings of the first study [Kim et al., 2015]. In these studies, Kim et al. el investigated the Ribonuclease A modifications induced by PBQ, 2-methyl-1,4-benzoquinone (MBQ), and 2-choro-1,4-benzoquinone (CBQ).

These tests were done using the same methods as the previous study, and they also used fluorescence, UV-Vis, SDS-PAGE, and microscopic imaging to measure protein modification. The results of this found that each quinone caused varying degrees of modification when incubated for the same amount of time. CBQ was found to be the most efficient in protein modification, followed by PBQ, and MBQ being the least efficient. LC-MS analysis also confirms the creation of adducts of quinone to protein and protein dimerization.

In another study presented as a Departmental Honors Thesis at UTC, Greve investigated the lysozyme modifications induced by PBQ, CBQ, and MBQ [Greve, 2015]. The study used the same concentrations as the previous studies, but only used SDS-PAGE to verify if any modifications of Lysozyme occurred. Since Lysozyme and Ribonuclease A have many similarities, the results were similar to the comparison study on Ribonuclease A and substituted PBQs where CBQ was found to be the most efficient in protein modification and MBQ being the least efficient. The only difference was the degree of oligomerization that each quinone induced.

Another experimental study was carried out by Smith, and it was also presented as a Departmental Honors Thesis at UTC. Smith investigated Ribonuclease A modifications when exposed to 1,2-naphthoquinone (ONQ) and 2-hydroxy-1,4-naphthoquinone (HNQ) [Smith, 2015]. For this study, the concentration of Ribonuclease A and naphthoquinones were both fixed at 0.10 mM and 5.0 mM, respectively. SDS-PAGE was primarily used to examine the Ribonuclease A modification through protein oligomerization induced by ONQ and HNQ. In addition, to better understand the effects of naphthoquinones on Ribonuclease A, the pH of Ribonuclease A was varied. The results showed that ONQ had a greater reactivity toward Ribonuclease A resulting in protein oligomerization. HNQ, on the other hand, did not cause

protein oligomerization regardless of pH. This led them to believe that protein modification occurred through other mechanisms.

Another study was carried out by Thomas, and it was given as a Departmental Honors Thesis at UTC. To add to Smith's study, Thomas investigated the modifications of Lysozymes and Ribonuclease A when exposed to a serious of benzoquinones and a few naphthoquinones using fluorescence and UV-Vis spectroscopy [Thomas, 2017]. Quinones used in his research are PBQ, MBQ, CBQ, tetrachloro-1,4- benzoquinone (TCBQ), phenyl-1,4-benzoquinone (PhBQ), HNQ, ONQ, and 1,4-naphthoquinone (PNQ). The reactions were carried out in a phosphate buffer (pH=7.0) at 37°C to mimic physiological conditions. Fluorescence spectroscopy was utilized to measure the degree of modification to the protein, and UV-Vis spectroscopy was used to monitor adduction formation and other protein modifications. The results showed that lysozyme modification through protein oligomerization and adduct formation increased with the concentration of PBQ, especially in the first three hours of incubations. In addition, with more electron withdrawing substituents on PBQ, the lysozyme modification was shown to increase. For the naphthoquinones investigated in this study, Lysozyme modification was found with all of them where ONQ seemed to elicit the largest degree of Lysozyme modification and HNQ with the least. This means that the reactivity of the naphthoquinones examined in this study were ONQ > PNQ > HNQ.

The last study presented here was given as a Departmental Honors Thesis at UTC and was done by Kurien. Kurien also investigated the modification of lysozyme by substituted benzoquinones and naphthoquinones [Kurien, 2018]. The benzoquinones examined in this study were PBQ, MBQ, PhBQ, CBQ, and TCBQ, while the naphthoquinones were ONQ, PNQ, and HNQ. While many of the experiments were performed at physiological conditions, there were

temperature dependence (27°C, 37°C, 42°C) and pH (6.0, 7.0, and 8.0) dependence reactions carried out as well. To visualize the protein modification, SDS-PAGE was used. The results showed that the substituted benzoquinones and naphthoquinones caused modifications at varying degrees, and the increase in temperature and pH caused an increase in protein modification as well. For the substituted benzoquinones examined, TCBQ was the most reactive, CBQ was second, PBQ was third, and MBQ was the least reactive. The naphthoquinones were all found to modify lysozyme at all conditions conducted in this study. From the results, the intensity of the aggregation was strongest for ONQ, then PNQ, and lastly HNQ. It was also noted that it was only a slightly greater aggregation between PNQ and HNQ. These result supports the findings of Thomas's study and suggest that ONQ is more reactive than PNQ, and PNQ is more reactivity than HNQ.

The study presented in this thesis will be a theoretical investigation on the reactivity of the naphthoquinones to complement Thomas' and Kurien's studies. Therefore, the results of Thomas' and Kurien's research on naphthoquinones will become an important source for comparison.

1.1.5 Prior theoretical studies on quinone reactivity

In our lab, quinone-related theoretical studies were carried out over many years. These studies were done to complement the experiments being conducted in lab as seen in the previous section. The quinones studied were *p*-benzoquinone, 2-chloro-*p*-benzoquinone, 2-methyl-*p*-benzoquinone and *o*-benzoquinone. In all studies mentioned below, computational calculations

were performed on *Gaussian 03* software using the hybrid density functional theory level mPW1B95-44 in conjunction with 6-31+G(d,p) basis set.

In an initial study carried out by Fernando, the reversible potential in gas-phase and aqueous phase were calculated for *p*-benzoquinone, 2-chloro-*p*-benzoquinone, 2-methyl-*p*-benzoquinone and *o*-benzoquinone [Fernando, 2009]. Fernando examined the nine possible reduction reactions for each of the selected quinones. A conformational analysis was carried out to find the minimum-energy species including quinone and anionic forms, semiquinone radical and anionic forms, and hydroquinone forms. In the presence of protons, all studied quinones have shown tendency to reduce to the respective hydroquinone by addition of two electrons and two protons in a single step in both gas and aqueous phases. Without the protons, reduction occurs by two single electron reduction steps in both phases. *o*-Benzoquinone had the highest reduction potentials and was considered the most prevailing oxidizing agent. With the substituents, chlorine was determined to enhance the reduction ability of PBQ while methyl substituents reduced its reduction ability.

In the other part of Fernando's study, the reactivity of the above mentioned four benzoquinone derivatives toward two nitrogen-containing nucleophiles, NH_3 and CH_3NH_2, and reactivity of *p*-benzoquinone toward two additional nitrogen-containing nucleophiles, $C_2H_5NH_2$ and lysine, were examined in the gas-phase [Fernando, 2009]. The study focused on the nucleophilic addition reactions at the carbonyl bonds. The reactions were investigated through three distinct pathways: a direct hydrogen transfer pathway, and two pathways involving the hydrogen transfer through a solvent, water or methanol. The results of this investigation confirmed that all the reactions are exothermic and the reactions are more likely to occur when they proceed via transition states involving solvent molecules like water or methanol. The

investigation also found that the barrier heights obtained for the amines and lysine are very close to each other and suggests that modeling the reaction can be done with smaller models like methylamine in place of biologically relevant molecules. This is important because all future studies will utilize methylamine to model a lysine amino acid from a protein. Like the first part of the study, *o*-benzoquinone was the most reactive of the quinones, and chlorine substituents enhancing the reactivity of PBQ while methyl substituents reducing reactivity.

Another investigation in our lab was carried out on the reaction between quinones and N-containing nucleophiles by Rathnayake. The quinones investigated were *p*-benzoquinone, chloro-*p*-benzoquinone, and methyl-*p*-benzoquinone, and the N-containing nucleophiles were ammonia, methylamine, and ethylamine. For the nucleophilic addition reactions, Rathnayake investigated if the hydrogen transfer was better through one water molecule or two water molecules. It was determined that the transfer of hydrogen was more favorable through two water molecules. To investigate the impact of using three different N-containing nucleophiles, he examined the barrier heights for *p*-benzoquinone with each of them. The results showed that the hydrogen substitution by alkyl group amine increase in reactivity, but the increased size of the substituted alkyl group only gives a slight rise to reactivity. These also reflect the results presented by Fernando. For all of the considered reaction paths, most of the transition states were optimized. In addition, possible reactant complexes where the reactants are in a trimer or tetramer complex were also examined to gain a better understanding of the overall reactions. Using all this information, the minimum reaction paths were identified for the investigated reactions. It was observed that reactant complexes, trimer or tetramer, can occur before the reaction goes through a transition state, and that all barrier heights were positive with respect to the complexes. This means that it might be better to start building a reaction pathway considering

these complexes instead of individual reactants as the zero of energy. The results of that study set the standards for how the research on naphthoquinones will be carried out.

1.1.6 Research Objective

As stated in the section 1.1.4, experimental research is currently being conducted on the reactivity of naphthoquinones on two proteins, Ribonuclease A and Lysozyme. To completement the research being conducted on naphthoquinones and further the knowledge on how the reaction is occurring, the study presented here will focus on the naphthoquinones utilized in the laboratory. The naphthoquinones of interest are 1,2-naphthoquinone, 1,4-naphthoquinone, and 2-hydroxy-1,4-naphthoquinone. In the computational study, the reactivity of these naphthoquinones will be investigated with a methylamine molecule, CH_3NH_2. The purpose of this study is to determine the reactivity of the various naphthoquinones toward an amino group by finding the most likely pathway for the reaction of each naphthoquinone to occur. This pathway will require the examination of the reactants, reactant complexes, transition states, and products in each reaction pathway. The calculated reactivities of the naphthoquinones will be compared to the experimental results to test for accuracy of the model. To our knowledge, similar investigations were done in our lab, but none in the literature.

1.2 Computational Methodologies

All electronic structure calculations were carried out using hybrid density functional theory (HDFT) method of mPW1B95-44 in conjunction with the 6-31+G(d,p) basis set which

was determined to give good results for transition state geometries [Zhao and Truhlar, 2004; Albu and Mikel, 2007]. All the geometry optimizations of products, reactants, and intermediate complexes including transition states were performed using a very tight convergence criterion and an ultrafine integration grid for numerical integrations. All the calculations were performed using *Gaussian 09* software [Frisch et al., 2009].

To better understand the HDFT method utilized for this experiment, a further breakdown of mPW1B95-44 is done. The mPW1B95-44 functional uses the modified Perdew-Wang (mPW) exchange functional [Adamo and Barone, 1998], followed by 1 indicating one parameter method, the B95 correlation functional [Becke, 1996], and a Hartree-Fock exchange contribution of 44%. This method was developed by Truhlar and Zhao and used to be known as MPWB1K. Truhlar and Zhao developed thus method to provide accurate results in determining barrier heights which gives good results for thermochemistry, thermochemical kinetics, hydrogen bonding, and weak interactions [Zhao and Truhlar, 2004]. In addition, this method was also shown to be very accurate in calculating properties including geometries, vibrational frequencies, enthalpies of formation, and NMR chemical shifts [De Silva and Albu, 2007].

For visualization of structures, ball and stick rendering is obtained by the Chemcraft software. In these structures, balls of white, gray, red, and blue represent hydrogen, carbon, oxygen, and nitrogen atoms, respectively. Figure 1.2 shows the rendering and color representation of the atoms used in the study. The connectivity between atoms are represented by sticks or cylinders, and intermolecular attractions like hydrogen bonding or van der Waals interactions are represented by dashed lines between the atoms. For this study, the term ‘conformer’ refers to non-optimized structures of products while ‘conformation’ refers to the optimized structures.

To have a better understanding of the spatial orientation of transition state geometries, four different perspectives will be given for certain conformations. These perspectives will be labeled α, β, γ, and δ. In the α perspective, the ten carbon atoms of the naphthoquinone ring are on a nearly vertical plane with the two carbonyl oxygen atoms on the vertical line. In the β perspective, all carbons in the naphthoquinone ring and the two carbonyl oxygens are on a nearly horizontal plane, and the viewer will see the two oxygen atoms nearly on top of each other with the amine group toward the viewer and above the horizontal plane. In the γ perspective, all carbons in the naphthoquinone ring and the two carbonyl oxygens are still on the horizontal plane, and the viewer will see the two oxygen atoms nearly on top of each other with the amine group away from the viewer and above the horizontal plane. Finally, the δ perspective has all the ring carbons and carbonyl oxygens are on a horizontal plane with the two carbonyl oxygens on a vertical plane. These perspectives are based on the 1,2-addition at carbonyl 1 of the 2-hydroxy-1,4-naphthoquinone reaction.

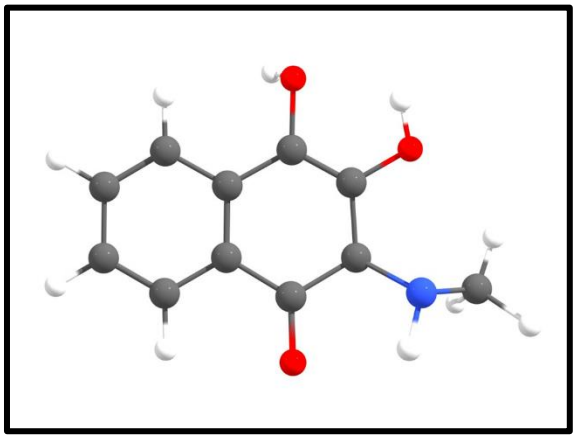


Figure 1.2 The rendering and color representation of 2-hydroxy-1,4-naphthoquinone utilized in the study

CHAPTER 2

REACTIVITY OF 2-HYDROXY-1,4-NAPHTHOQUINONE

2.1 Introduction

As stated in section 1.1.6, the purpose of this study is to investigate the N-containing nucleophilic addition for selected naphthoquinones by carrying out electronic structure theory computations in the gas-phase. The first reaction investigated was the first step of the reaction between 2-hydroxy-1,4-naphthoquinone or 2-hydroxy-*para*-naphthoquinone (HNQ) and methylamine, CH_3NH_2. Figure 2.1 depicts the numbering of the carbon atoms on HNQ throughout this study. For the reaction between HNQ and CH_3NH_2, there are four different product isomers that can be formed since there are two unique carbonyl positions and two possible reactions for each carbonyl position. The two unique carbonyl positions are at position 1 and position 4 (Figure 2.1). Therefore, the possible reactions are a 1,2-addition at carbonyl 1 (C1), a 1,4-addition at C1, a 1,2-addition at carbonyl 4 (C4), or a 1,4-addition at C4. Figure 2.2 depicts a general schematic for the possible product isomers that can be formed from the reaction of 2-hydroxy-1,4-naphthoquinone and CH_3NH_2. All the possible reactions studied for the reaction of HNQ and CH_3NH_2, namely 1,2-addition at C1, 1,4-addition at C1, 1,2-addition at C4, and 1,4-addition at C4, are shown in Figures 2.3, 2.4, 2.5, and 2.6, respectively. For each reaction pathway, there are few stages of reaction namely reactants, reactant complexes, transition states, and products that must be examined to understand the overall reactivity of the naphthoquinone toward an amino group. Each of the reactions are labeled **R-Hx** where R stands

for reaction, H stands for hydroxyl-naphthoquinone, and x=1-4 stands for each possible reaction path. Similarly, the four products are labeled **P-Hx** where P stands for product.

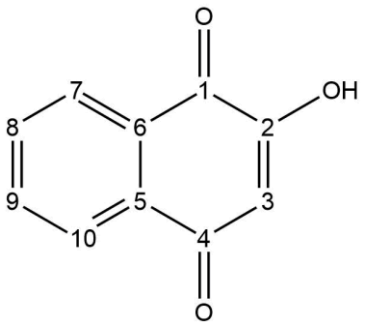


Figure 2.1 Carbon centers numbering of 2-hydroxy-1,4-naphthoquinone

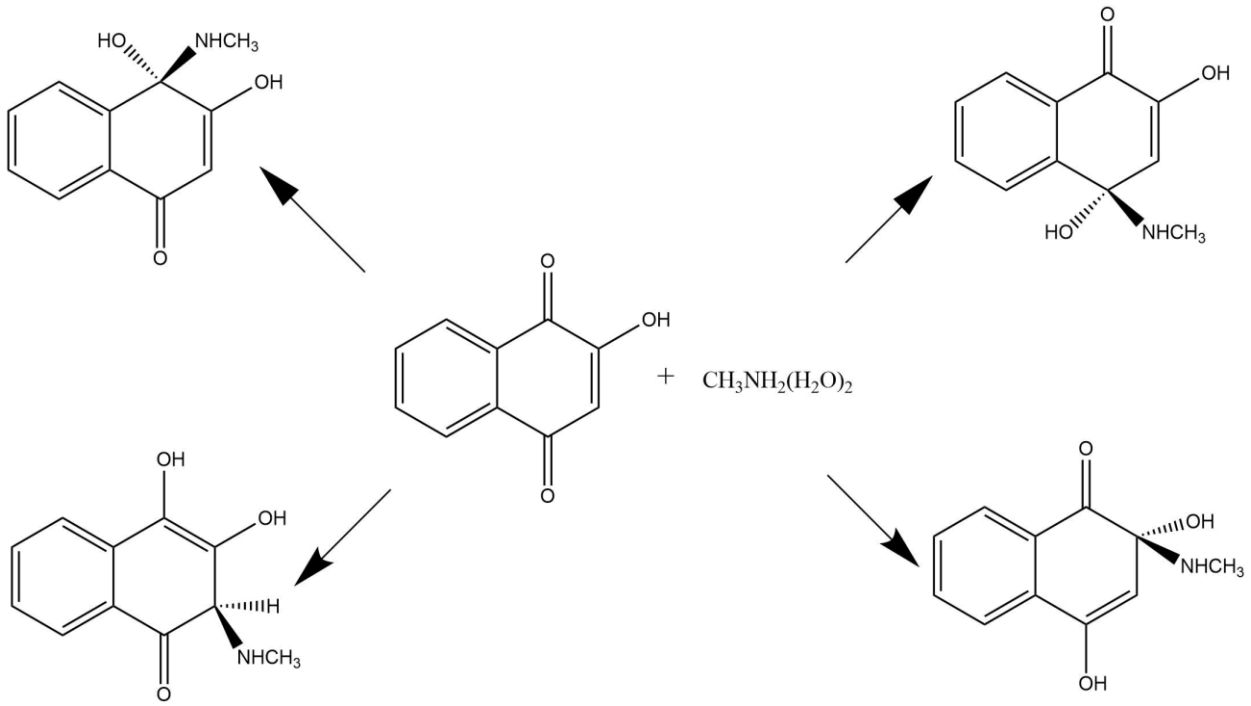


Figure 2.2 Possible reaction pathways for 2-hydroxy-1,4-naphthoquinone and CH_3NH_2

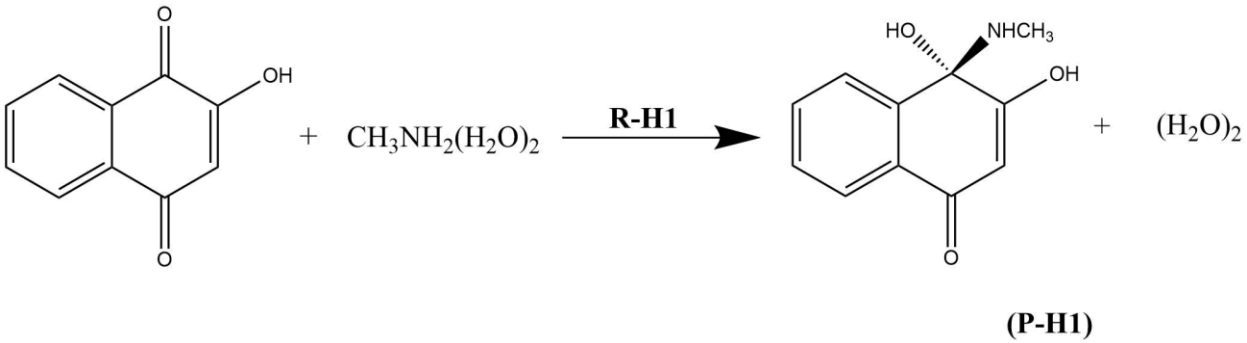


Figure 2.3 1,2-Addition between 2-hydroxy-1,4-naphthoquinone and CH_3NH_2 at position 1

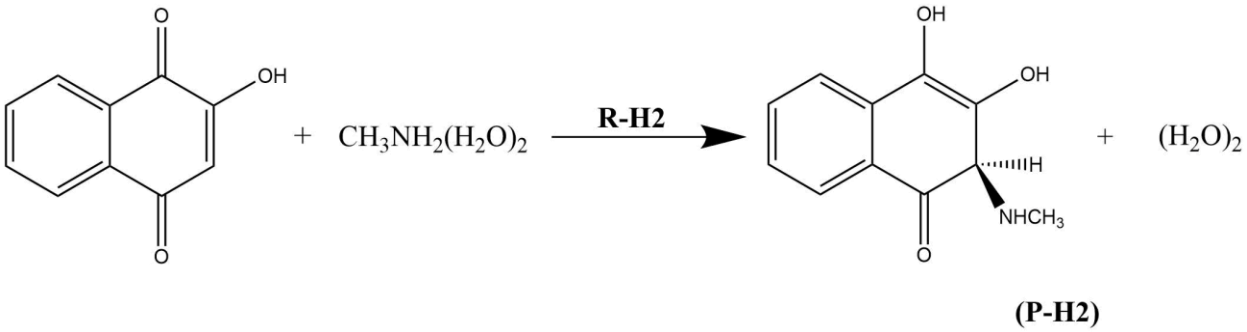


Figure 2.4 1,4-Addition between 2-hydroxy-1,4-naphthoquinone and CH_3NH_2 at position 1

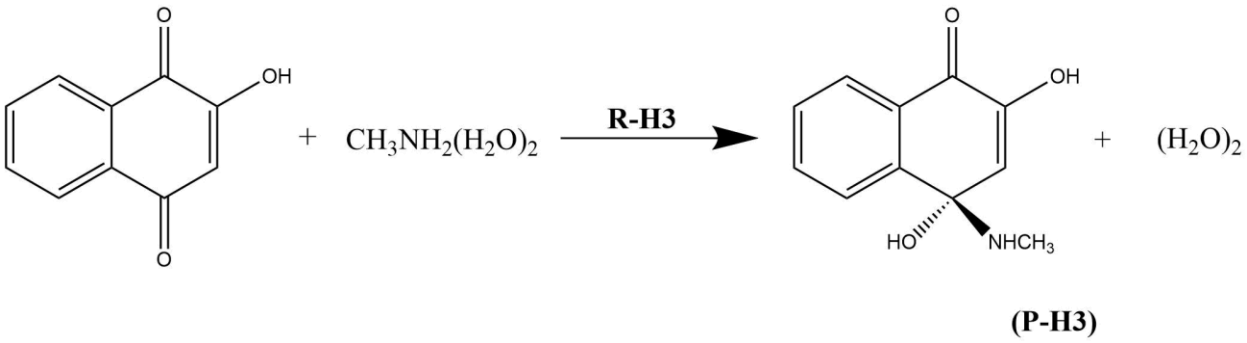


Figure 2.5 1,2-Addition between 2-hydroxy-1,4-naphthoquinone and CH_3NH_2 at position 4

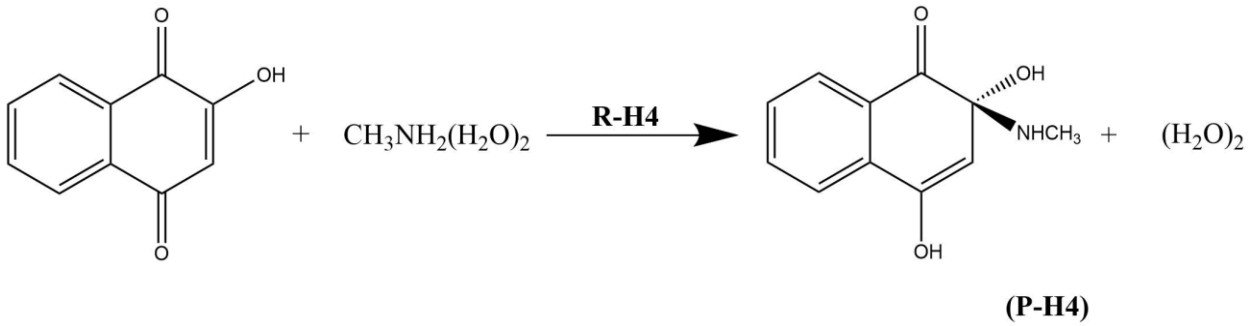
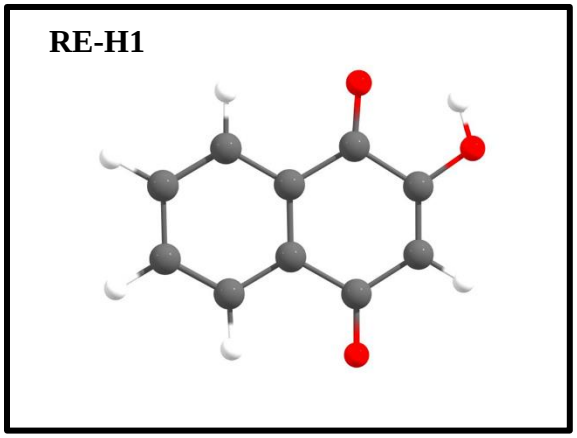


Figure 2.6 1,4-Addition between 2-hydroxy-1,4-naphthoquinone and CH_3NH_2 at position 4

2.2 Structure and properties of the reactant state (2-hydroxy-1,4-naphthoquinone)

2.2.1 Hydroxynaphthoquinone as a reactant

For all reaction pathways examined in this study, there must be a point of reference to compare the energy of each structure with that of another structure. Therefore, each stage of reactions in this study must have a reference energy value to compare to which, for this study, will be the energy values of the reactants. The first part of the reactant state will always be the naphthoquinones of interest, and for Chapter 2, this reactant is HNQ. HNQ is unique in that it can exist as two isomers, 2-hydroxy-1,4-naphthoquinone or 4-hydroxy-1,2-naphthoquinone. For each isomer, the OH position can be rotated around the C–O bond which leads to different conformers. A total of four different conformations were modeled and optimized. The reactants for HNQ are labeled **RE-Hx** where RE stands for reactant state, H stands for HNQ, and x is a number to specify a different conformation. The four optimized structures are shown in Figures 2.7 and 2.8.



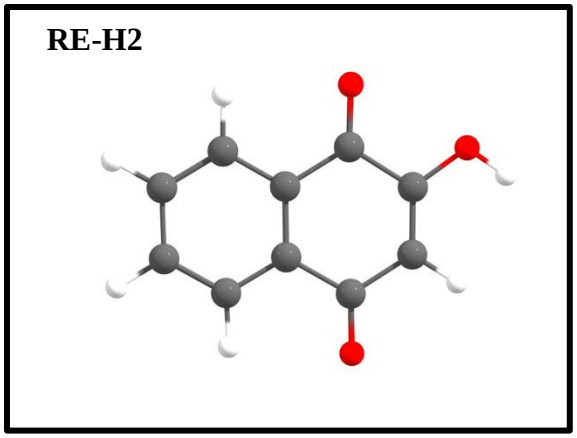
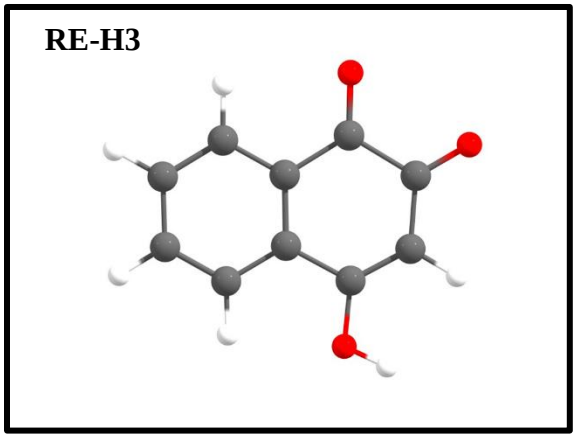


Figure 2.7 **RE-H1** and **RE-H2**: Optimized structures of 2-hydroxy-1,4-naphthoquinone



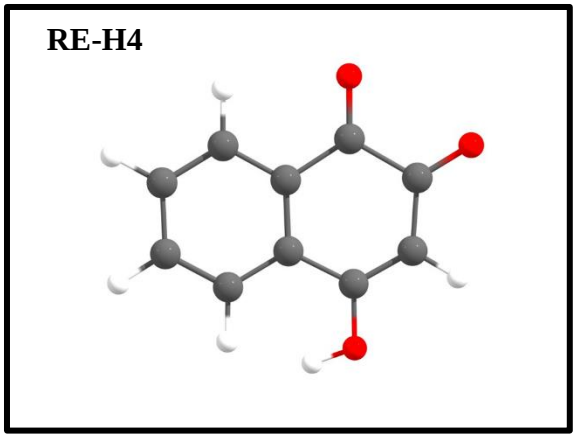


Figure 2.8 **RE-H3** and **RE-H4**: Optimized structures of 4-hydroxy-1,2-naphthoquinone

Among the four reactant conformations, **RE-H1** was determined to be the most stable structure and will be utilized as part of the energy for the reactants. The relative energies of **RE-H2**, **RE-H3**, and **RE-H4** with respect to **RE-H1** are 7.05 kcal/mol, 11.31 kcal/mol, and 16.29 kcal/mol, respectively.

2.2.2 $2H_2O$-CH_3NH_2 Trimer as a reactant

Aside from the naphthoquinones studied in each chapter, the other remaining reactant part is the two water molecules utilized for the hydrogen transfer and methylamine. There are two ways that one could examine the remaining reactants. One is to calculate them separately and add up their individual energies, and the other way is to calculate them as a complex for a single energy value. The possible complexes for the reactants are water dimers – $(H_2O)_2$, two water molecules and methylamine trimers - $2H_2O$-CH_3NH_2 trimers, and two water molecules, methylamine, and naphthoquinone tetramers - $2H_2O$-CH_3NH_2-naphthoquinone tetramers. Rathnayake has already examined the utilization of the dimer and trimer complexes and compared them to their individual energy values. It was determined that utilizing the remaining reactants as a trimer allows for the best results where one gets positive values for the gas-phase barrier heights. In a previous study, 10 different orientations were examined and optimized using HDFT of mPW1B95-44 in conjunction with 6-31+G(d,p) basis set, and only three different orientations for the trimer complex were determined [Rathnayake, 2013]. This study utilized the data from Rathnayake's study and also obtained three distinct structures from five different initial structures of the reactant complex. The three optimized structures are shown in Figure 2.9.

Of the three optimized orientations of trimer complexes, T-a was determined to be the most stable conformation and will be utilized as the other stage for the energy for the reactants. The relative energies of T-b and T-c relative to T-a are 0.05 kcal/mol and 0.19 kcal/mol, respectively. The difference in relative energy with respect to each other is small overall, which means that the other orientations could occur. Unlike HNQ, it should be noted that this structure

does not change for the other reactions examined in the other chapters of this study and will be utilized in all chapters for relative energy determinations.

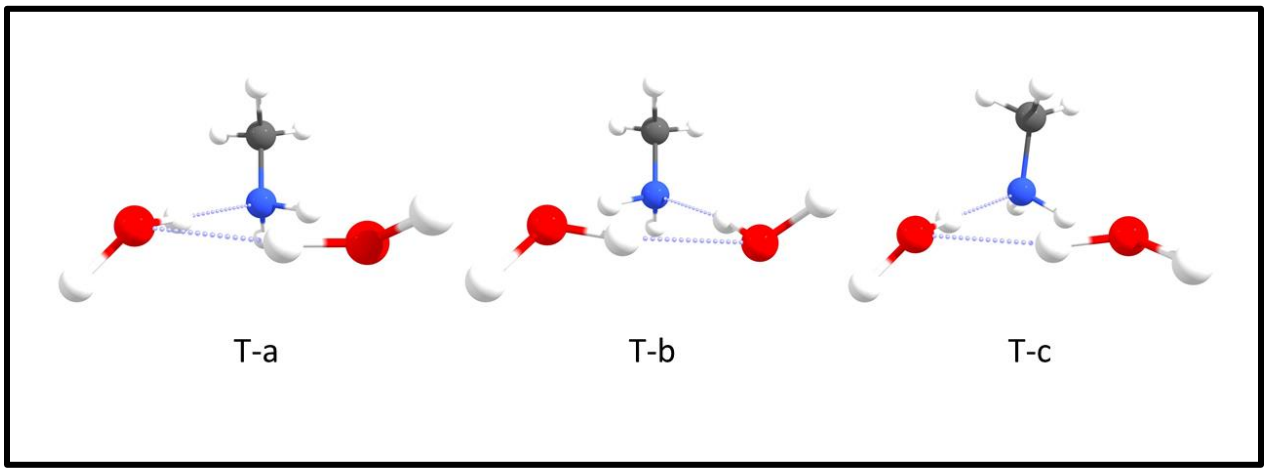


Figure 2.9 T-a, T-b, and T-c: Optimized orientations of trimer complexes (methylamine and two water molecules)

2.2.3 Reactant complexes

Along the reaction pathway, there is also the possibility of considering the complex including all the reactants as the reference energy. In this case, the two water molecules, methylamine and a 2-hydroxy-1,4-naphthoquinone would form a tetramer. These tetramer complexes would be interesting because they would account for the interactions of all the reactants. By having all the interactions, one could more accurately represent the reaction in solution. Overall, 26 different possible arrangements of the 2-hydroxy-1,4-naphthoquinone tetramer were investigated with only 13 unique optimized conformations found. The lowest energy tetramer was determined and depicted in Figure 2.10. Other interesting tetramers are shown in Figure 2.11 and give a good idea of how the molecules within the tetramer like to

orient. It should be noted that there are many ways for the tetramer to form, and it would be difficult to examine all possibilities. Each of these calculations took anywhere from three to eleven days of computation on one processor to determine an optimized structure. The reactant complexes for HNQ are labeled **RC-Hx** where RC stands for reactant complex, H stands for HNQ, and x is a number to specify a different conformation. The reactant complexes are labeled from lowest energy to greatest energy, but not all structures are shown here. Only some interesting tetramers are shown in Figure 2.11, so there will be gaps in the labeling of the tetramers. The remaining tetramers' structures can be found in the appendix.

For the tetramer complex, **RC-H1** was determined to be the most stable structure of the tetramer complex. When compared to 2-hydroxy-1,4-naphthoquinone and the trimer of the reactants, **RC-H1** had a relative energy of -9.14 kcal/mol. The relative energies of **RC-H2**, **RC-H5**, **RC-H6**, **RC-H8**, **RC-H9**, **RC-H10**, **RC-H11**, and **RC-H12** in Figure 2.11 with respect to **RC-H1** are 1.52 kcal/mol, 2.32 kcal/mol, 4.69 kcal/mol, 5.11 kcal/mol, 5.52 kcal/mol, 6.70 kcal/mol, 6.71 kcal/mol, and 7.69 kcal/mol, respectively.

By comparing the optimized orientations and their respective energies, there seems to be a trend with how the reactants orient themselves. As seen in **RC-H1**, **RC-H2**, and **RC-H5**, the energy of the complex is generally lower when the two water molecules and methylamine are interacting with one another. This might suggest that the two water molecules and methylamine form a trimer more readily than interacting individually with the naphthoquinone. In addition, the other complexes support this by having a higher energy when one molecule is away from the rest of the original trimer.

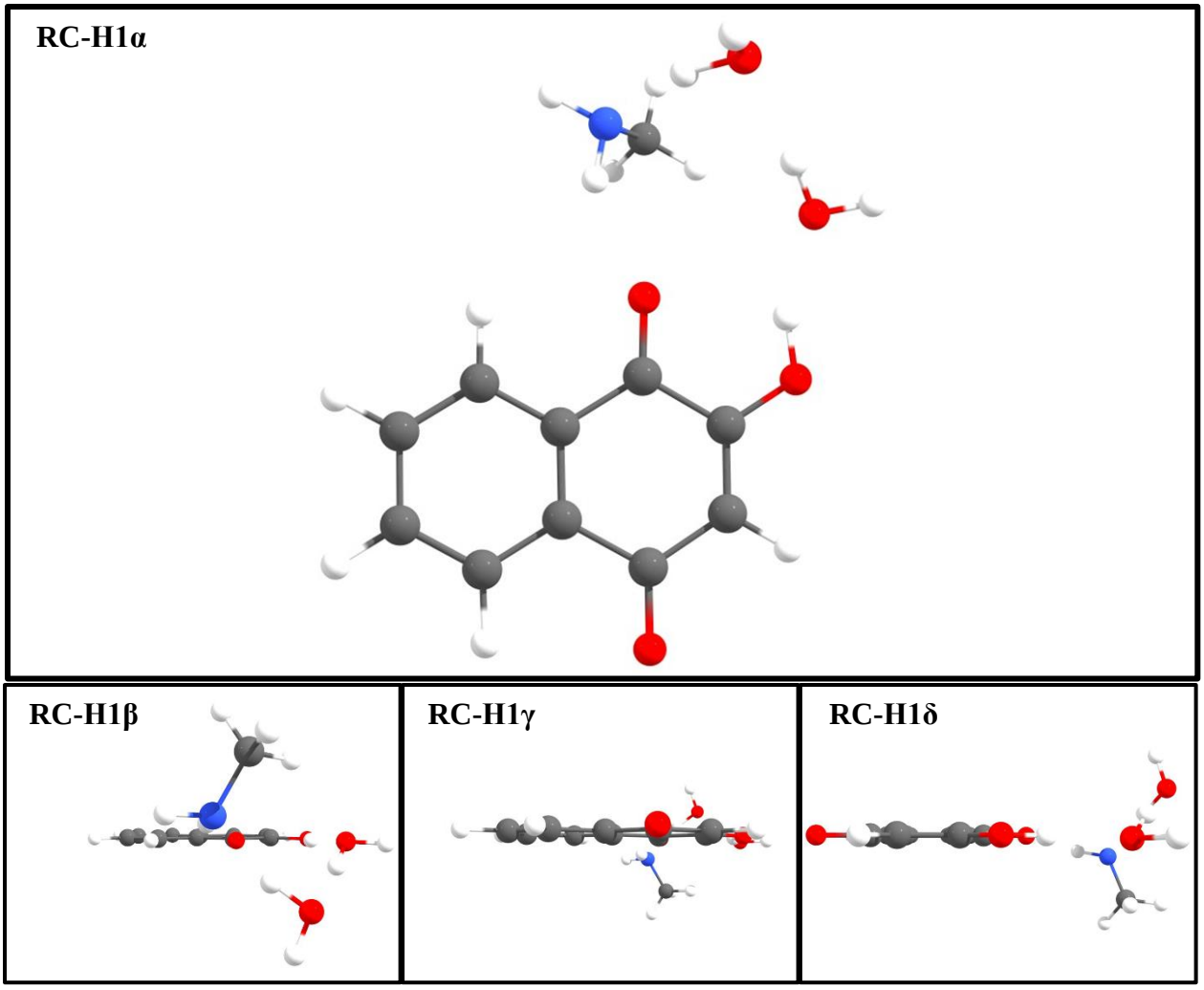
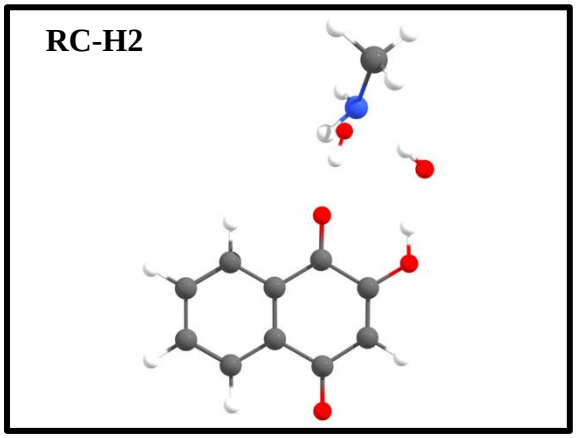
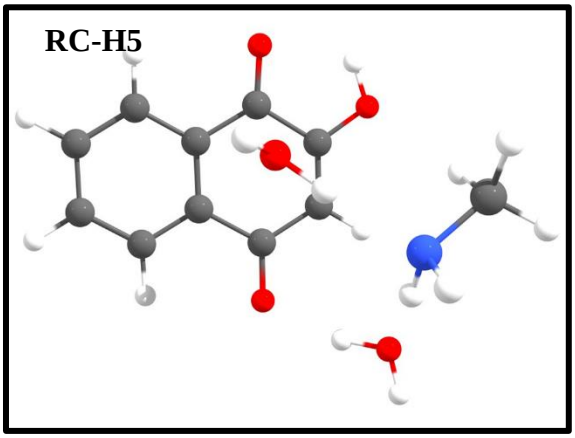


Figure 2.10 Optimized orientation of most stable tetramer complex (2-hydroxy-1,4-naphthoquinone, methylamine, and two water molecules)





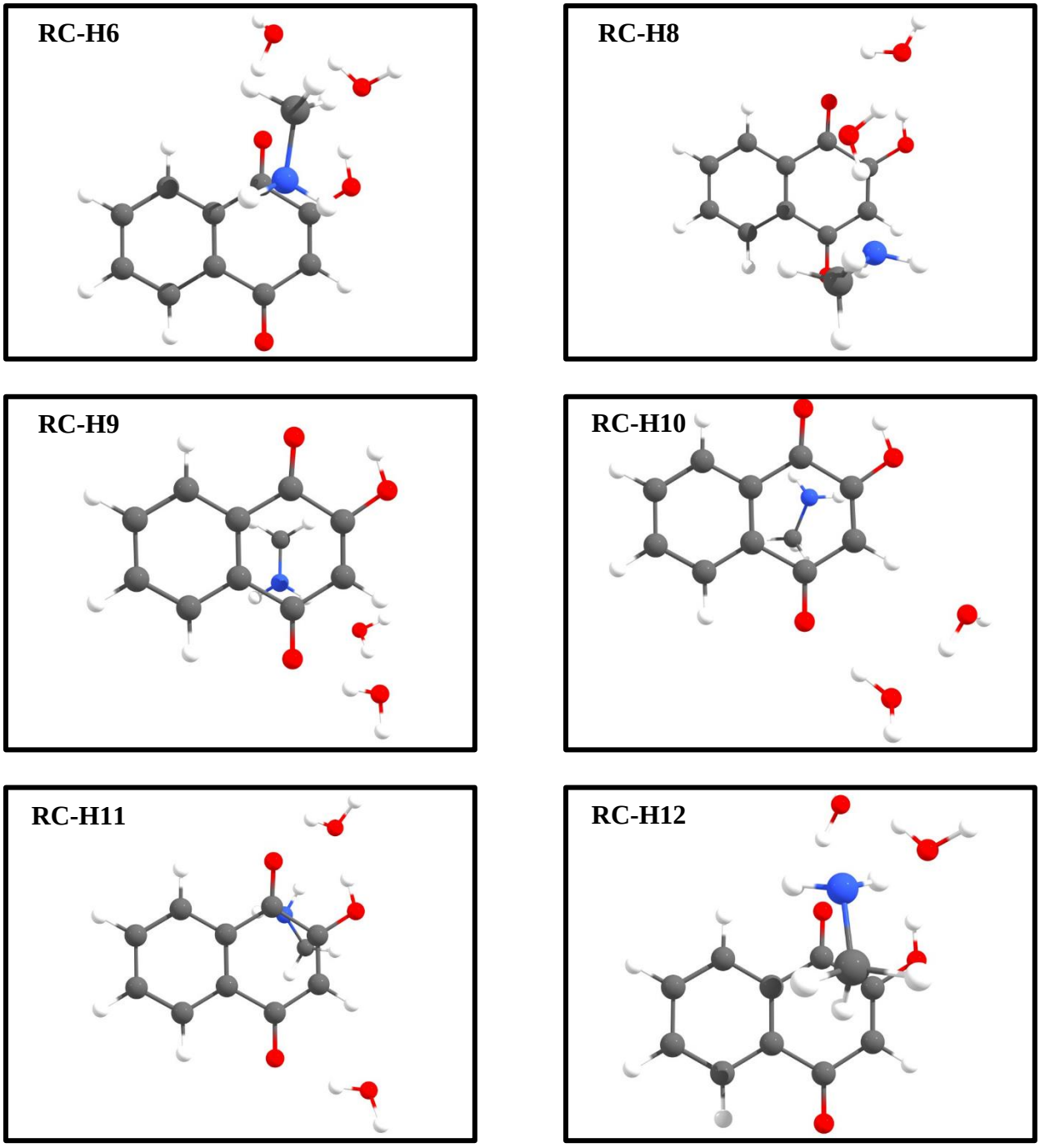


Figure 2.11 Optimized orientations of other tetramer complexes (2-hydroxy-1,4-naphthoquinone, methylamine, and two water molecules)

2.3 Structure and properties of the product state

2.3.1 2-Hydroxy-1,4-naphthoquinone and CH_3NH_2 products

The next stage of the reaction between 2-hydroxy-1,4-naphthoquinone and methylamine depicted in Figure 2.2 is finding the most stable structures of the reaction products. A detailed conformation analysis was carried out for the products in Figure 2.2 where there are 90 possible product conformers based on the four possible reactions. Each reaction makes a combination of 24 possible orientations for the 1,2-additions and 21 possible orientations for the 1,4-additions. Each product will have a different IUPAC name, but the factors examined will be the same. The factors examined in these possible conformers are the orientation of the two OH functional groups, one that was already on 2-hydroxy-1,4-naphthoquinone ring and the other that formed from the single H atom addition, and the methyl and hydrogen orientation on the binding methylamine. The bound methylamine has a single bond which allows for rotation around the C–N bond, and this rotation was also examined. The calculation time for the optimized geometry of a product conformation is around one to two days. From the 90 possible conformers, 74 distinct product conformations were optimized. Figures 2.12, 2.13, 2.14, and 2.15 represent the four lowest energy products from **R-H1**, **R-H2**, **R-H3**, and **R-H4** reactions, respectively. As stated previously in section 2.1**, P-Hx_1-x_2** where P stands for product, H stands for HNQ, x_1=1-4 stands for each possible reaction path mentioned in section 2.1, and x_2 stands for a different conformation.

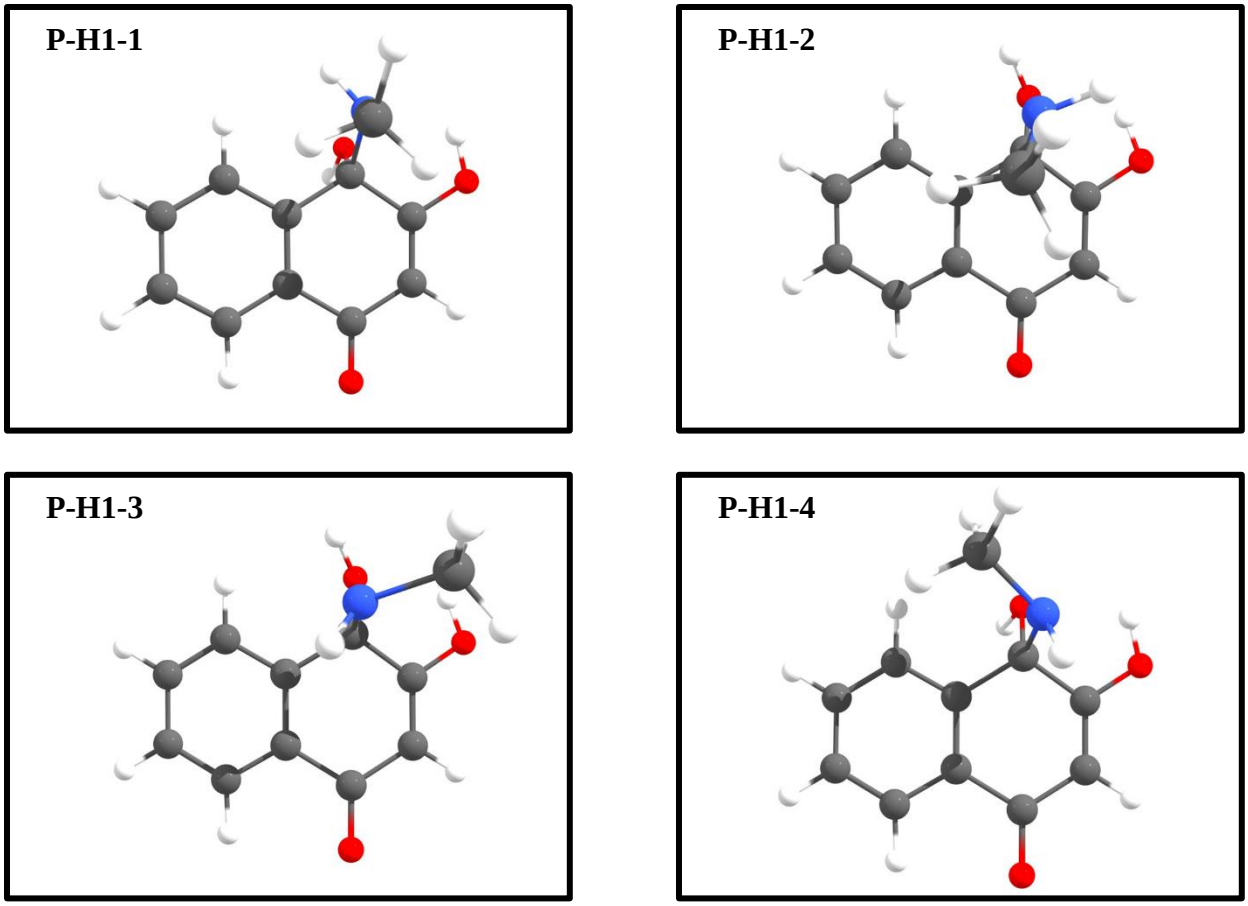


Figure 2.12 **P-H1-1**, **P-H1-2**, **P-H1-3**, and **P-H1-4**: Four lowest energy structures for the product of **R-H1** reaction

Among the four product conformations in Figure 2.12, **P-H1-1** was determined to be the most stable structure for the product of the **R-H1** reaction. The relative energies of **P-H1-2**, **P-H1-3**, and **P-H1-4** with respect to **P-H1-1** are 0.76 kcal/mol, 1.40 kcal/mol, and 2.02 kcal/mol, respectively. For the products of **R-H1**, 21 conformations were optimized, and the least stable conformation has a relative energy of 8.77 kcal/mol.

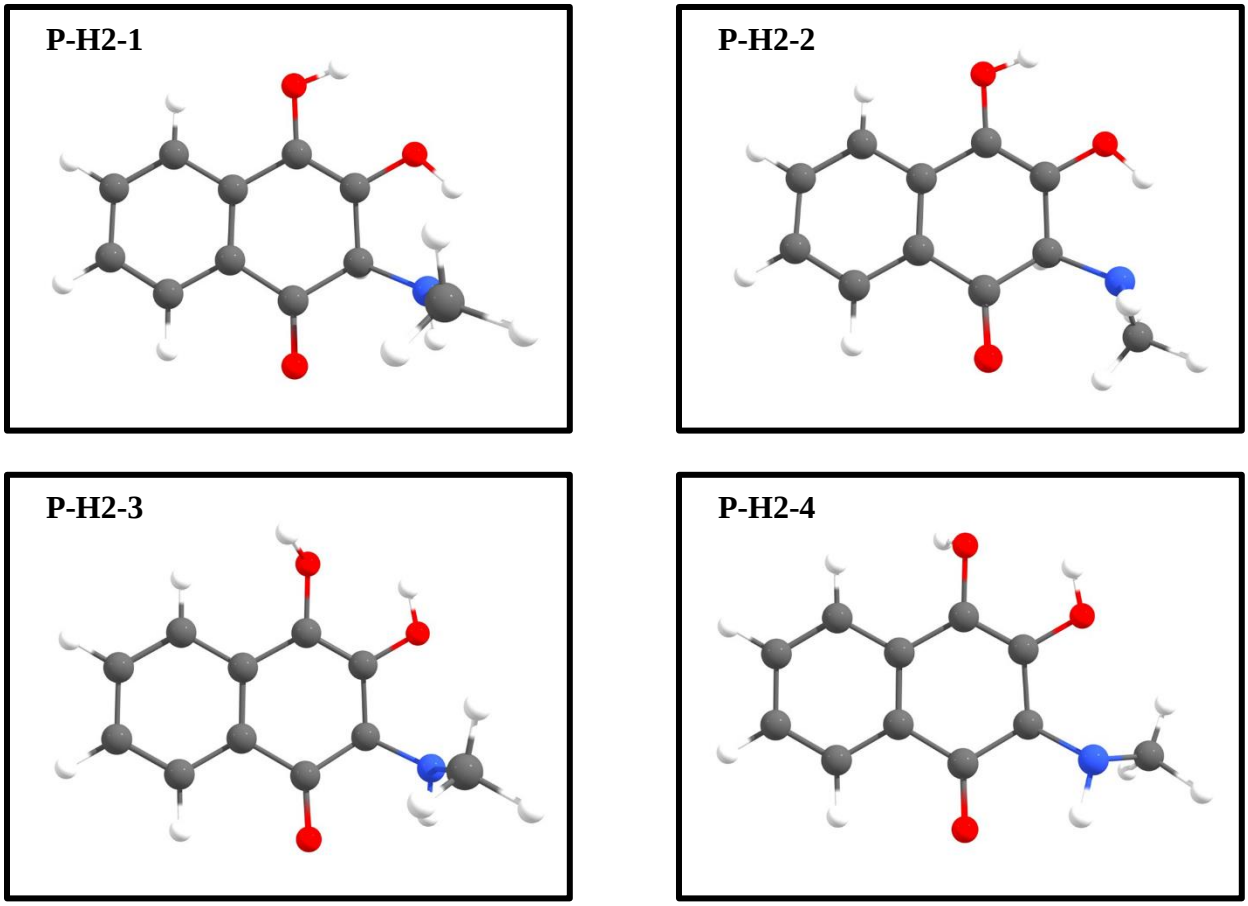


Figure 2.13 **P-H2-1**, **P-H2-2**, **P-H2-3**, and **P-H2-4**: Four lowest energy structures for the product of **R-H2** reaction

Among the four product conformations in Figure 2.13, **P-H2-1** was determined to be the most stable structure for the product of the **R-H2** reaction. The relative energies of **P-H2-2**, **P-H2-3**, and **P-H2-4** with respect to **P-H2-1** are 0.54 kcal/mol, 7.34 kcal/mol, and 7.42 kcal/mol, respectively. For the products of **R-H2**, 13 conformations were optimized, and the least stable conformation has a relative energy of 15.15 kcal/mol.

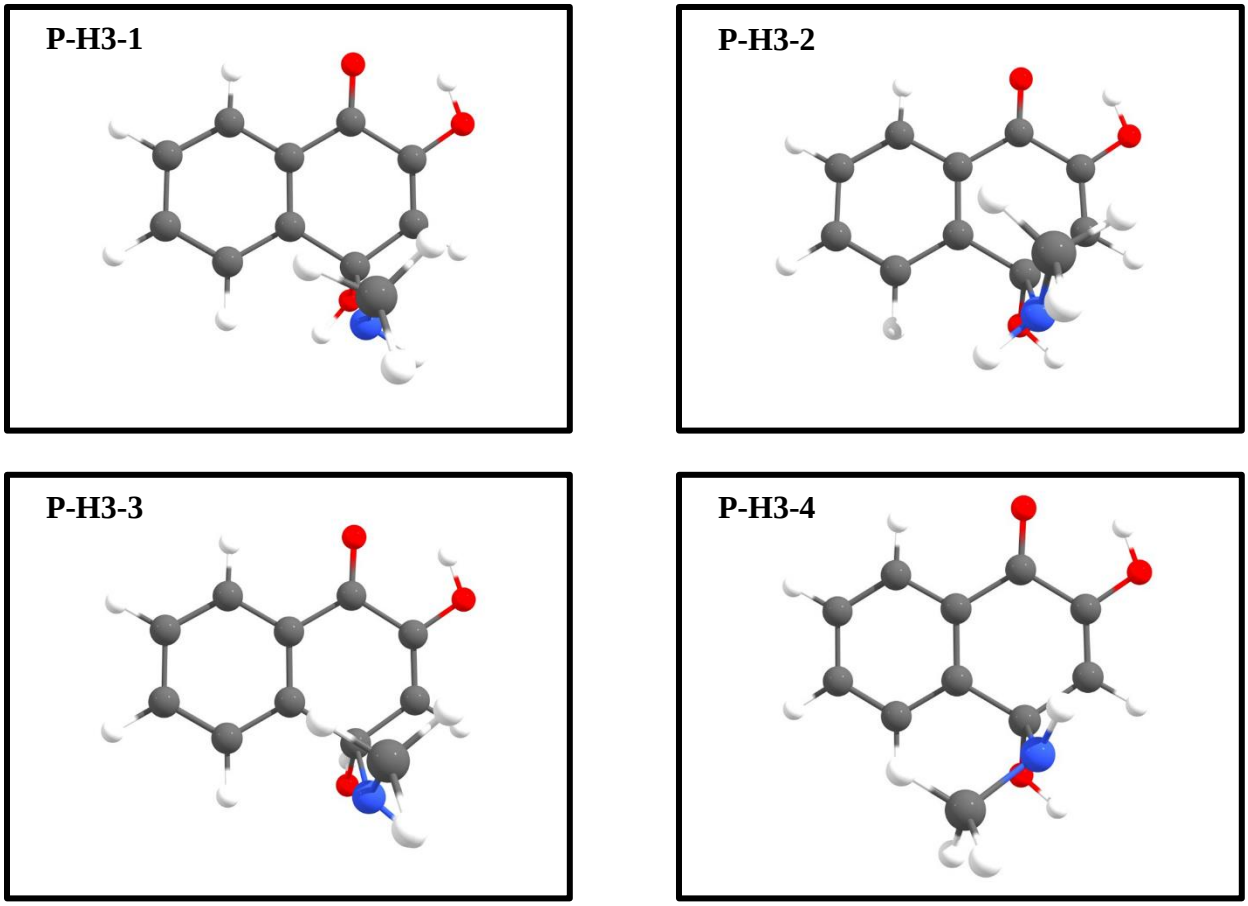


Figure 2.14 **P-H3-1**, **P-H3-2**, **P-H3-3**, and **P-H3-4**: Four lowest energy structures for the product of **R-H3** reaction

Among the four product conformations in Figure 2.14, **P-H3-1** was determined to be the most stable structure for the product of the **R-H3** reaction. The relative energies of P **P-H3-2**, **P-H3-3**, and **P-H3-4** with respect to **P-H3-1** are 0.06 kcal/mol, 0.62 kcal/mol, and 0.92 kcal/mol, respectively. For the products of **R-H3**, 24 conformations were optimized, and the least stable conformation has a relative energy of 11.77 kcal/mol.

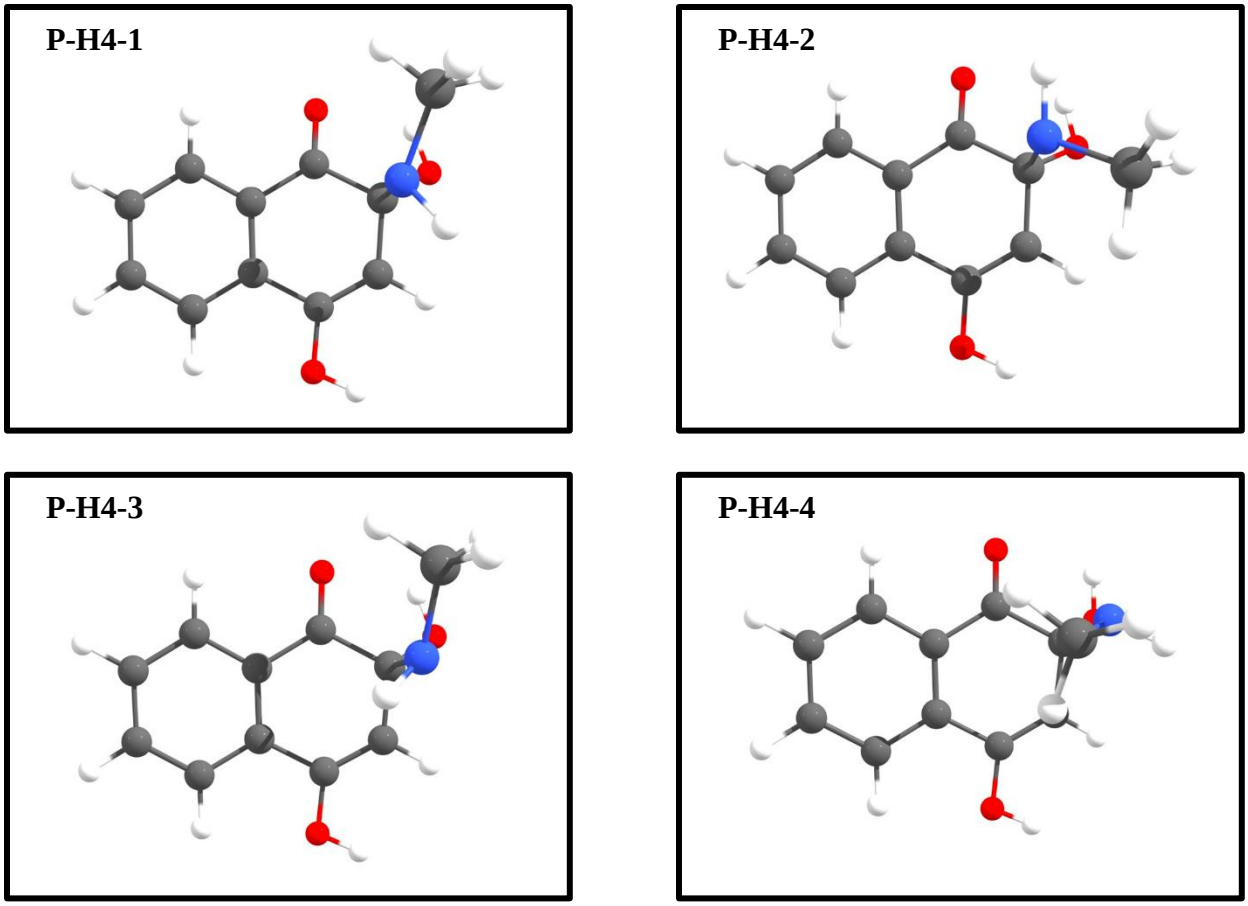


Figure 2.15 **P-H4-1**, **P-H4-2**, **P-H4-3**, and **P-H4-4**: Four lowest energy structures for the product of **R-H4** reaction

Among the four product conformations in Figure 2.16, **P-H4-1** was determined to be the most stable structure for the product of the **R-H4** reaction. The relative energies of **P-H4-2**, **P-H4-3**, and **P-H4-4** with respect to **P-H4-1** are 0.01 kcal/mol, 0.92 kcal/mol, and 1.65 kcal/mol, respectively. For the products of **R-H4**, 16 conformations were optimized, and the least stable conformation has a relative energy of 9.04 kcal/mol.

2.3.2 Water dimer as a product

After the formation of the main product, the water molecules utilized in our model to facilitate the hydrogen transfer are left over and have to be accounted for. For the water molecules, it would be fine to just add their individual energies to the product, but like the reactants, it would not give an accurate representation of the reaction. It would be better to treat the water molecules as a complex like in section 2.2 where the reactants were treated as complexes. It would be too time consuming and is not significant enough to examine all the products together as a trimer, so this study considers the two water molecules as a dimer and adds the energy onto the major product.

Anderson and Tschumper have characterized the potential energy surfaces of 10 different conformations of water dimer complexes (Figure 2.17) with 10 different density functional theory methods [Anderson and Tschumper, 2006].

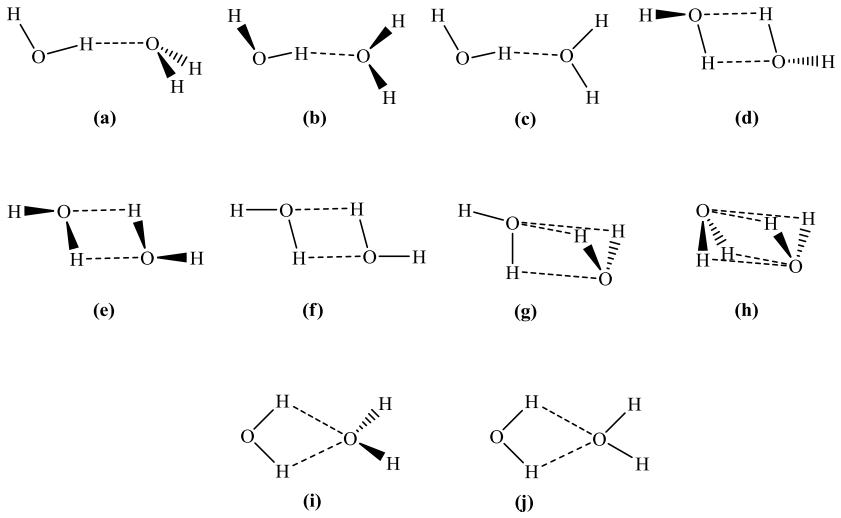


Figure 2.16 Ten possible orientations of water dimers. Adapted from Anderson and Tschumper, 2006

In a previous study, six geometries (structures a to f from Figure 2.16) from the above publication were examined and optimized using the HDFT and basis set that are also utilized in this study (mPW1B95-44/6-31+G(d,p)). Rathnayake determined that structure a in Figure 2.16 is the most stable structure from the considered water dimers, and this water dimer will be utilized for the product energy in this study [Rathnayake, 2013]. The optimized geometry of the water dimer used in this study is seen in Figure 2.17.

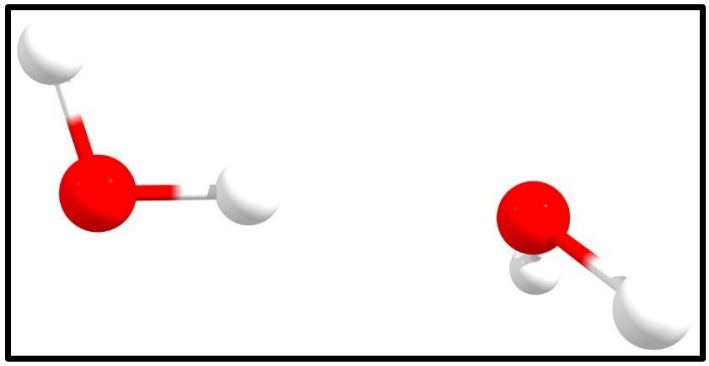


Figure 2.17 Optimized structure of water dimer used in study

2.4 Analysis of transition states

The transition state is the most important stage of the reaction pathway because it determines the energy barrier that must be overcome for the reaction to occur. Therefore, it is necessary to determine the most likely transition state for each possible reaction pathways so that one can determine which reaction is most likely to occur. In this study, there will be a focus on the first step of the hydrogen transfer from the nucleophile, methylamine, to the carbonyl group at carbon 1 and 4 of 2-hydroxy-1,4-naphthoquinone as the transition state. To study these transition states, one must decide how the hydrogen transfer will be modeled. Fernando

examined three of the ways for the hydrogen transfer to occur: a direct hydrogen transfer, the transfer through methanol, or the transfer through water. It was determined that the gas-phase barrier height was much higher for the direct hydrogen transfer compared to the two solvents that were similar in energy [Fernando, 2009]. These results mean that either solvent would be a good model for the hydrogen transfer, and since the reaction in the lab is in a water solvent, using water would be better as a model. Based off the previously mentioned study, Rathnayake utilized the assistance of two water molecules to model the hydrogen transfer in his transition states, and this model will be utilized as the foundation for the naphthoquinones of interest during this study [Rathnayake, 2013].

An analysis was carried out for the transition states of 1,2-addition at C1, 1,2-addition at C4, 1,4-addition at C1, and 1,4-addition at C4. The important factors examined in each transition state in this section are the OH position on the quinone ring, the methyl position on the amine, the location of the hydrogen transfer through the two water molecules (only for the 1,2-addition reactions), and the position of the hydrogens on the two water molecules. There was a total of 68 transition states examined, and only 36 distinct conformations were optimized as transition states. Overall, the calculation times for the optimized geometry of a transition state ranges from two to four days. As for the naming of the structures presented in this study, **TS-Hx$_1$-x$_2$** where TS stands for transition state, H stands for HNQ, x_1=1-4 stands for each possible reaction path mentioned in section 2.1, and x_2 stands for a different conformation in that possible reaction path. The labeling was done where it starts from the lowest energy structure to the highest energy structure. The labeling of the atoms in the transition state is depicted in Figure 2.18, and this labeling will be utilized generally for all transition states. The only difference between

naphthoquinones is the location of the oxygen on the carbonyl. This will only occur for 1,2-naphthoquinone where the oxygen labeled O_4 will become O_2 and will be on the second carbon.

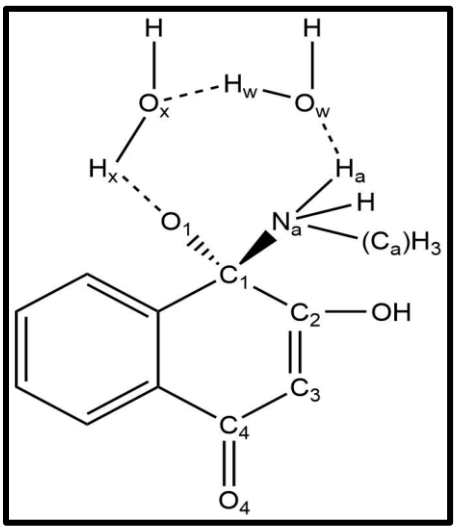


Figure 2.18 General labeling of atoms for the transition state

2.4.1 1,2-Addition at carbonyl 1 of 2-hydroxy-1,4-naphthoquinone

Twenty-one different conformers of the transition state were examined, and only thirteen distinct transition states were identified for the **R-H1** reaction. A summary of some important parameters of the transition states are given in Tables 2.1 and 2.2. The symbols $V^{\ddagger}$ and $\omega^{\ddagger}$ are gas-phase barrier height in kcal/mol and imaginary frequency in cm^{-1}, respectively. The gas-phase barrier height in the tables of this section are relative to energy of the individual naphthoquinone and $CH_3HN_2(H_2O)_2$ trimer energy values. For Table 2.2, the intermolecular distances presented in the table are in angstroms (Å).

There were some interesting observations for the four lowest energy transition states. In **TS-H1-1**, **TS-H1-2**, **TS-H1-3**, and **TS-H1-4,** two steps were taken for the hydrogen transfer

processes to occur, and these two steps were broken into what we called an early and late transition state. After examining the early and late transition states, it was determined that the early transition state is where the hydrogen from the O_x of the second water has already transferred, while the H_a from the methylamine has just started to move. Then, the late transition state has the transfer of the remaining hydrogens on the methylamine and the first water occur at the same time. To have a better understanding of these early and late states, a general model of where the hydrogens are in the transition state can be seen in Figure 2.19. For the labeling of the early and late transition states of this study, **a** will be added to the previously mentioned transition state labeling to represent the early state, and **b** will be added to represent the late transition state. As seen in Table 2.1, it was determined that the early transition states had a lower gas-phase barrier height than the late transition states. In addition, since the early and late transition states are describing the same reaction pathway, only one of them will be used to represent the energy barrier along the reaction coordinate. For this study, the late transition states must be utilized for each distinct conformation because it represents the higher-energy barrier height.

The four lowest transition states with their early and late states were determined and depicted in Figures 2.20-2.27. These figures will give a better depiction of the two different states. The front views of the remaining distinct transition states are depicted in Figures 2.28 and 2.29. As shown in Table 2.1, **TS-H1-1b** has the lowest gas-phase barrier height of 4.50 kcal/mol when compared to the reactants, 2-hydroxy-1,4-naphthoquinone and the $CH_3HN_2(H_2O)_2$ trimer. Transition states **TS-H1-1b** to **4b** only have a range of 2 kcal/mol between them which means that they could all occur. It is just that **TS-H1-1** is the more likely to occur.**TS-H1-13** was

determined to have the greatest gas-phase barrier height of 18.66 kcal/mol and was determined to not likely occur.

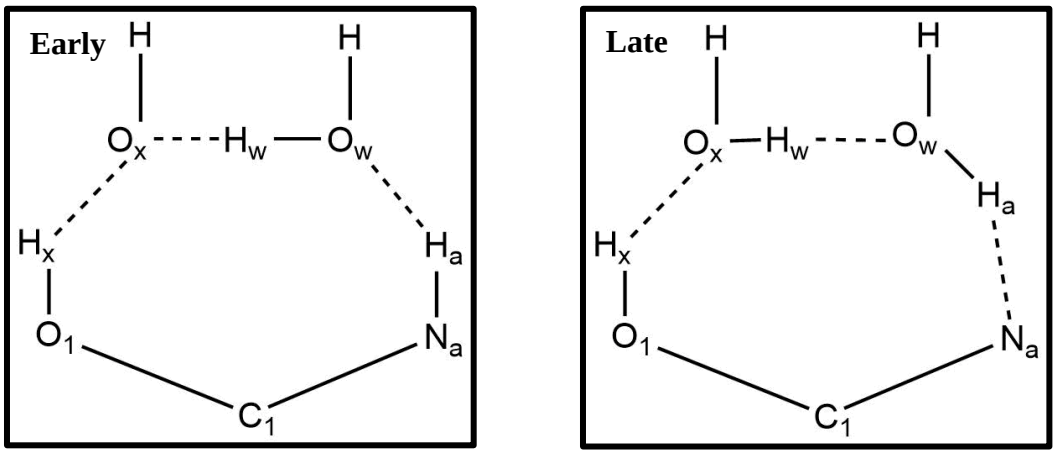


Figure 2.19 General model for early and late transition states of **R-H1** reaction

When changing orientation of methylamine group, there tends to be a variation in the gas-phase barrier height around 0.6 kcal/mol in these structures. For example, transition state **TS-H1-1b**, where the methyl group is pointing forward as seen in Figure 2.21, has a barrier height of 4.50 kcal/mol while transition state **TS-H1-2b**, where the methyl group is pointing toward the side as seen in Figure 2.23 (all other atoms are in similar positions), has a barrier height of 5.12 kcal/mol.

Next, when changing the orientation of hydrogens on the two water molecules, there is less than a 1 kcal/mol variation to total gas-phase barrier height. For example, transition state **TS-H1-1b**, where the hydrogen on the first water is pointing to the right and the hydrogen on the second water is pointing more to the left as seen in Figure 2.21, has a barrier height of 4.50 kcal/mol while transition state **TS-H1-3b**, where the hydrogen on the first water is pointing to

the left and the hydrogen on the second water is pointing more to the right as seen in Figure 2.25 (all other atoms are in similar positions), has a barrier height of 5.27 kcal/mol.

Table 2.1 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-H1**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-H1-1a	2.45	618*i*
TS-H1-1b	4.50	1018*i*
TS-H1-2a	2.63	569*i*
TS-H1-2b	5.12	1031*i*
TS-H1-3a	3.25	627*i*
TS-H1-3b	5.27	1005*i*
TS-H1-4a	3.99	528*i*
TS-H1-4b	6.60	1001*i*
TS-H1-5	8.06	1177*i*
TS-H1-6	8.59	1145*i*
TS-H1-7	9.96	1145*i*
TS-H1-8	13.93	1285*i*
TS-H1-9	16.68	928*i*
TS-H1-10	16.76	710*i*
TS-H1-11	17.29	945*i*
TS-H1-12	18.59	699*i*
TS-H1-13	18.66	754*i*

When moving the location of the water pathway for the hydrogen transfer over the naphthoquinone ring, there tends to be a variation in the gas-phase barrier height by 4-5 kcal/mol. For example, transition state **TS-H1-1b**, where the water path is away from the naphthoquinone ring as seen in Figure 2.21, has a barrier height of 4.50 kcal/mol while transition

state **TS-H1-6**, where the water path is over the naphthoquinone ring as seen in Figure 2.25 (all other atoms are in similar positions), has a barrier height of 8.59 kcal/mol.

The last factor examined was changing the orientation of the hydroxyl on HNQ, and there tends to be a wide variation in the gas-phase barrier height ranging from 10 to 14 kcal/mol. For example, transition state **TS-H1-1b**, where hydroxyl point towards the water path as seen in Figure 2.21, has a barrier height of 4.50 kcal/mol while transition state **TS-H1-8**, where the hydroxyl points away from the water path as seen in Figure 2.25 (all other atoms are in similar positions), has a barrier height of 13.93 kcal/mol.

Table 2.2 Selected internuclear distances (Å) for transition state of reaction **R-H1**

Transition State	C_1—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_1—H_x	C_1—O_1
TS-H1-1a	1.584	1.041	1.736	0.984	1.670	1.215	1.168	1.328
TS-H1-1b	1.522	1.176	1.321	1.164	1.219	1.620	0.990	1.367
TS-H1-2a	1.592	1.041	1.732	0.986	1.663	1.230	1.153	1.323
TS-H1-2b	1.527	1.178	1.320	1.168	1.216	1.608	0.991	1.360
TS-H1-3a	1.589	1.039	1.748	0.984	1.667	1.216	1.168	1.328
TS-H1-3b	1.524	1.172	1.328	1.168	1.215	1.644	0.986	1.369
TS-H1-4a	1.594	1.037	1.742	0.985	1.661	1.241	1.144	1.324
TS-H1-4b	1.529	1.170	1.328	1.172	1.211	1.622	0.987	1.361
TS-H1-5	1.530	1.159	1.344	1.166	1.221	1.298	1.109	1.348
TS-H1-6	1.533	1.148	1.360	1.163	1.222	1.297	1.111	1.352
TS-H1-7	1.534	1.146	1.361	1.177	1.210	1.304	1.105	1.348
TS-H1-8	1.535	1.150	1.367	1.160	1.230	1.236	1.161	1.335
TS-H1-9	1.555	1.110	1.445	1.146	1.253	1.325	1.099	1.330
TS-H1-10	1.544	1.111	1.439	1.125	1.272	1.360	1.075	1.334
TS-H1-11	1.545	1.122	1.418	1.143	1.255	1.324	1.095	1.333
TS-H1-12	1.542	1.108	1.453	1.135	1.258	1.395	1.055	1.338
TS-H1-13	1.550	1.106	1.443	1.131	1.265	1.359	1.076	1.333

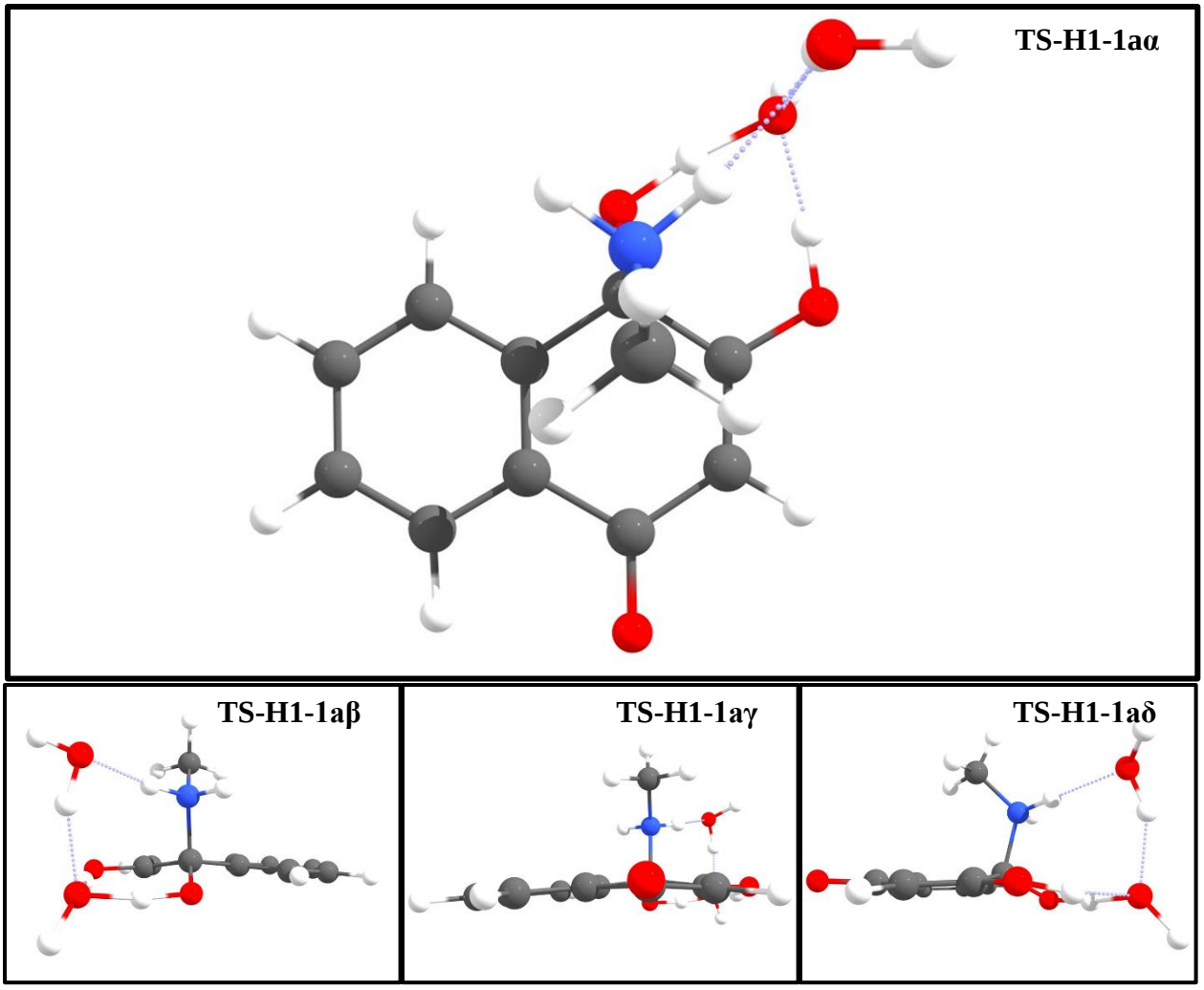


Figure 2.20 Transition state **TS-H1-1a** (early transition state of **TS-H1-1)**

Since the **R-H1** reaction has the possibility to form early and late transition state, the intermolecular distances must be examined in two parts. According to Table 2.2, intermolecular distances C_1–N_a, N_a–H_a, O_w–H_w, O_1–H_x, and C_1–O_1 in early transition states have comparatively consistent values around 1.590 Å, 1.040 Å, 0.985 Å, 1.158 Å and 1.326 Å, respectively, for all the structures. In comparison, the intermolecular distances C_1–N_a, N_a–H_a, O_w–H_w, O_1–H_x, and C_1–O_1 in the late transition states have comparatively consistent values around 1.526 Å, 1.174 Å, 1.168 Å, 0.9885 Å and 1.364 Å, respectively. When comparing the intermolecular distances, it

can be seen how far the hydrogen transfer has gone and allows us to separate the early and late states. The C_1–N_a in the early states are longer than the late states while the N_a–H_a is shorter in comparison. This seems to reflect that the hydrogen has not started its transfer in the early transition state when compared to the late transition state. This also depicts how methylamine is further away from the naphthoquinone ring in the early transition state.

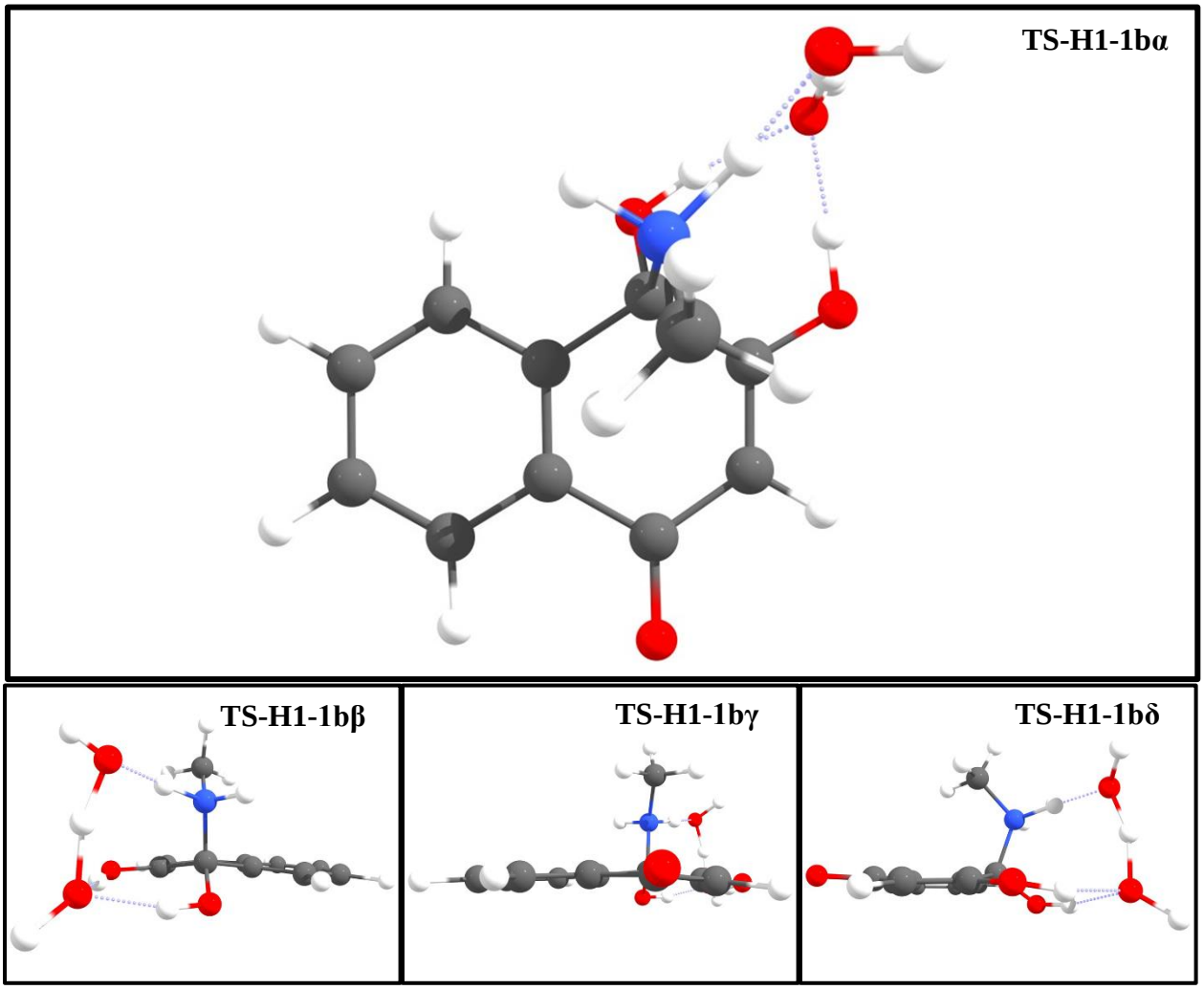


Figure 2.21 Transition state **TS-H1-1b** (late transition state of **TS-H1-1**): Lowest energy structure for transition state of **R-H1** reaction

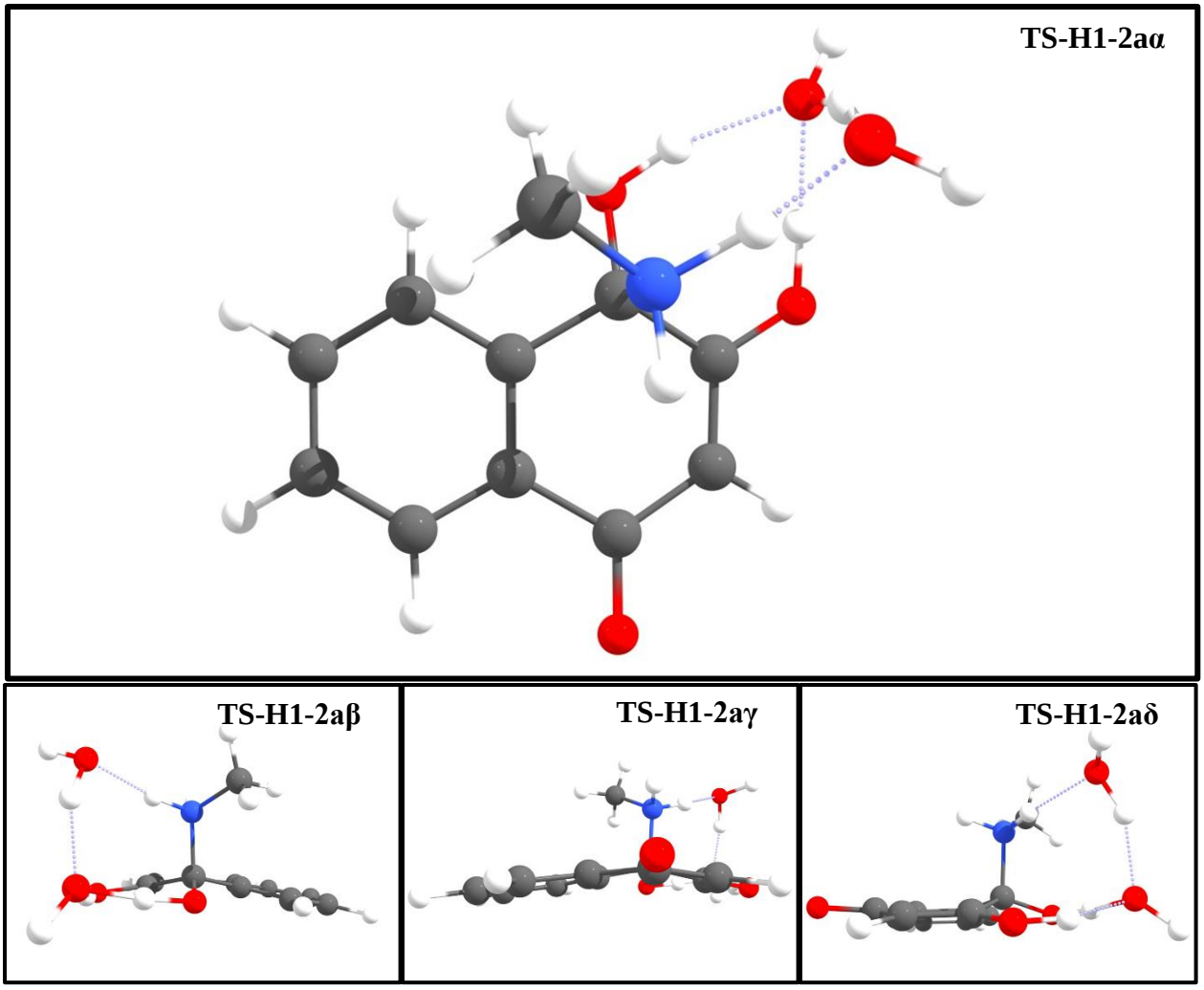


Figure 2.22 Transition state **TS-H1-2a** (early transition state of **TS-H1-2**)

Next, the O_w–H_w intermolecular distance as seen in Table 2.2 is shorter in the early transition states when compared to the late transition states. This means that the hydrogen of the first water molecule is still bonded to its oxygen and has not really started the transfer to the oxygen in the second water of the model. The intermolecular distance O_1–H_x is longer in the early transition state and describes how the hydrogen from the second water has not fully transferred to the oxygen on the naphthoquinone ring. This also means that the late transition state has already completed this hydrogen transfer as described previously. The C_1–O_1

intermolecular distance in the early transition states are shorter when compared to the early transition states, and this would reflect that the atoms have more double bond character in the early transition state compared to the late transition state. For the remaining transition states of the **R-H1** reaction, the intermolecular distances N_a–H_a, O_1–H_x, and C_1–O_1 have comparatively consistent values around 1.129 Å, 1.098 Å, and 1.339 Å, respectively. The remaining intermolecular distances had wide ranges and were not consistent.

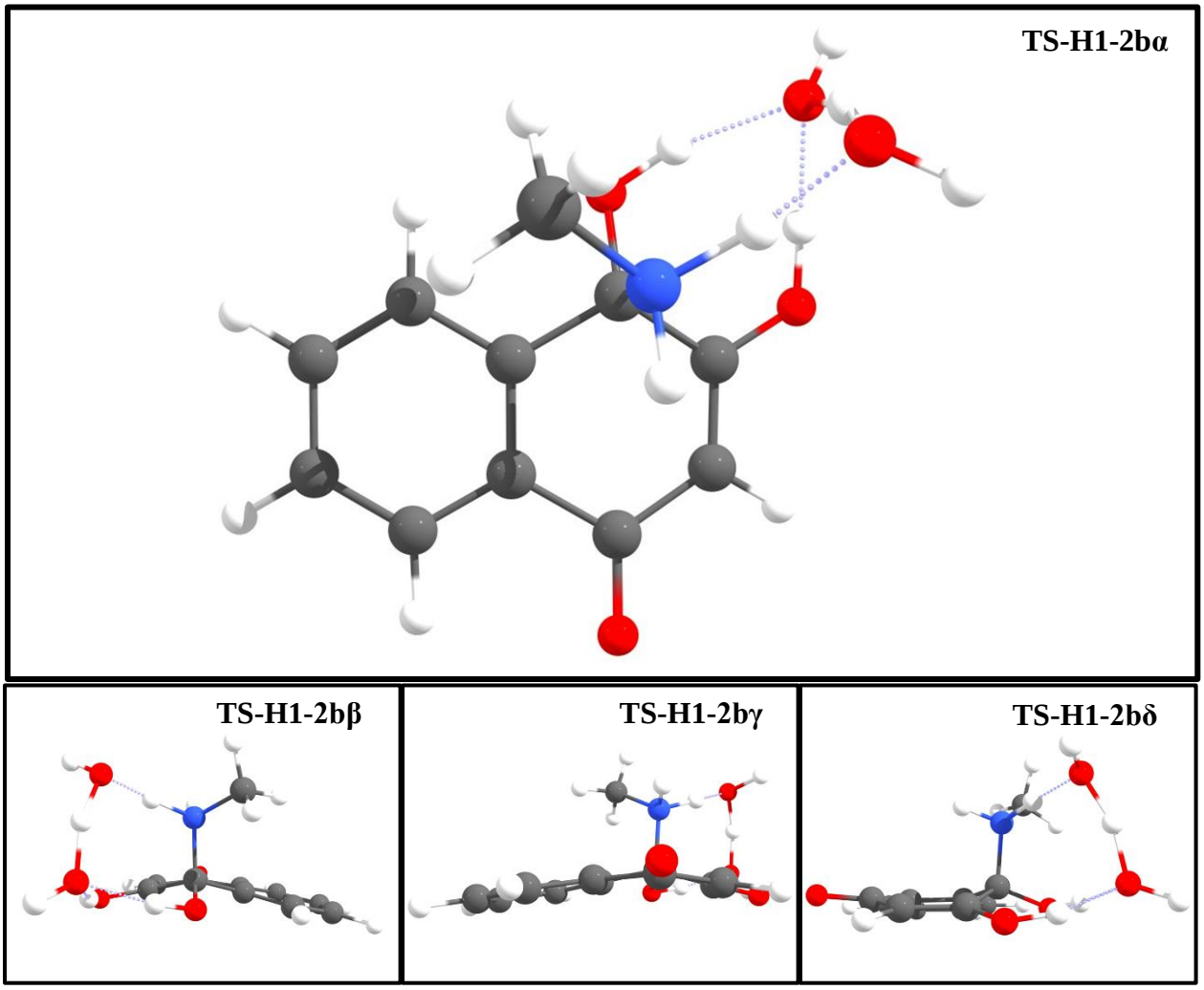


Figure 2.23 Transition state **TS-H1-2b** (late transition state of **TS-H1-2**)

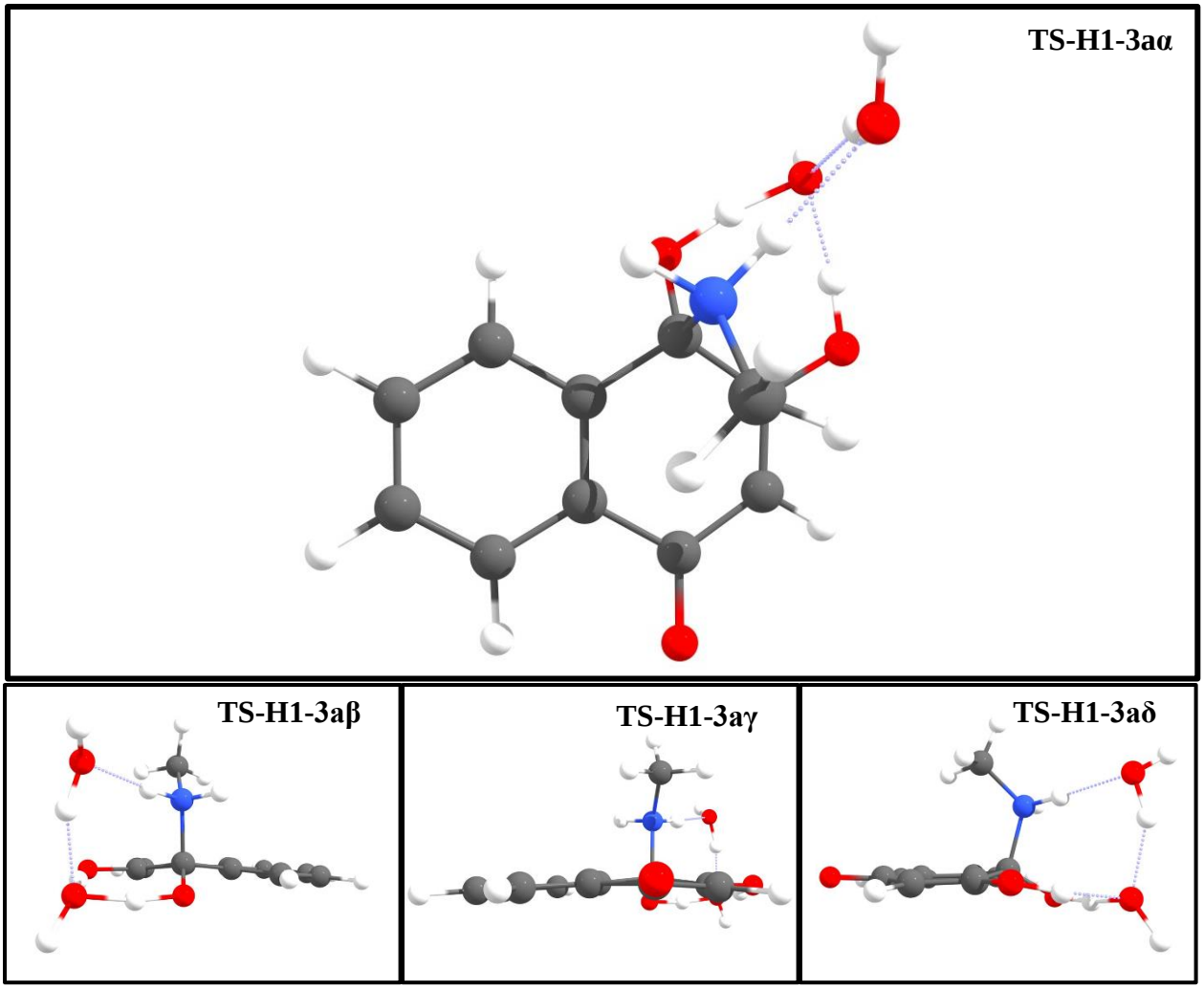


Figure 2.24 Transition state **TS-H1-3a** (early transition state of **TS-H1-3**)

The imaginary frequencies are within a wide range of 528*i* cm^{-1} and 1285*i* cm^{-1}. A small imaginary value implies a wide barrier while a large imaginary value implies a narrow barrier. As for trends in the structures, the early transition states tend to have lower imaginary frequencies in the 500*i*-600*i* cm^{-1} range. This imaginary frequency involves mainly the motion of H_x between O_x and O_1. The late transition states tend to have higher imaginary frequencies around 1000*i* cm^{-1}. For these transition states, the atoms involved in the imaginary frequency are H_a and H_w. The motion of atoms involved in the imaginary frequency is consistent with the

motion of atoms described early based on internuclear distances. For structures with the water pathway over the naphthoquinone ring, the imaginary frequencies tend to be around 1100*i* cm^{-1} to 1200*i* cm^{-1}. The orientation of the hydroxyl does not seem to have a trend in its imaginary frequency.

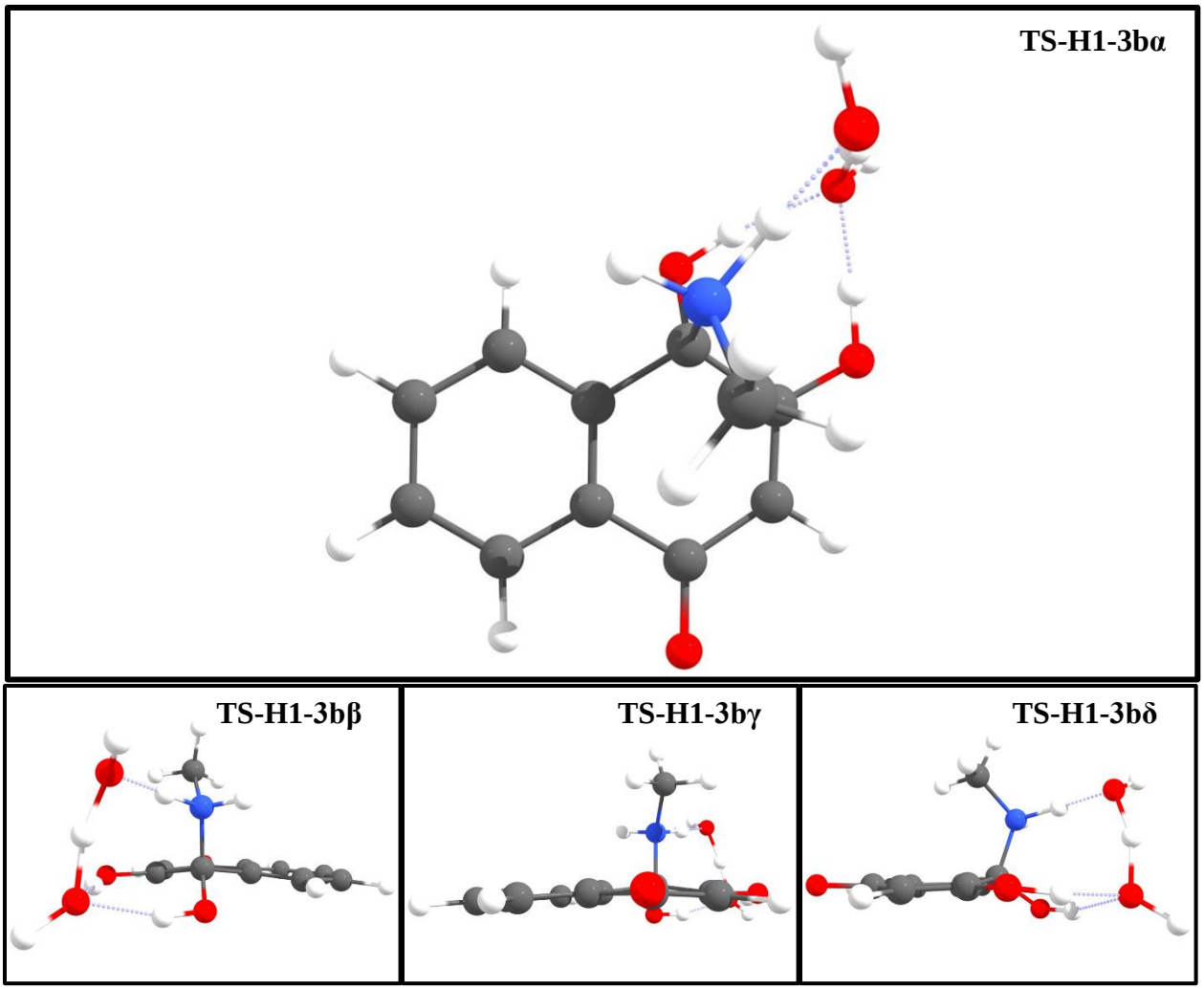


Figure 2.25 Transition state **TS-H1-3b** (late transition state of **TS-H1-3**)

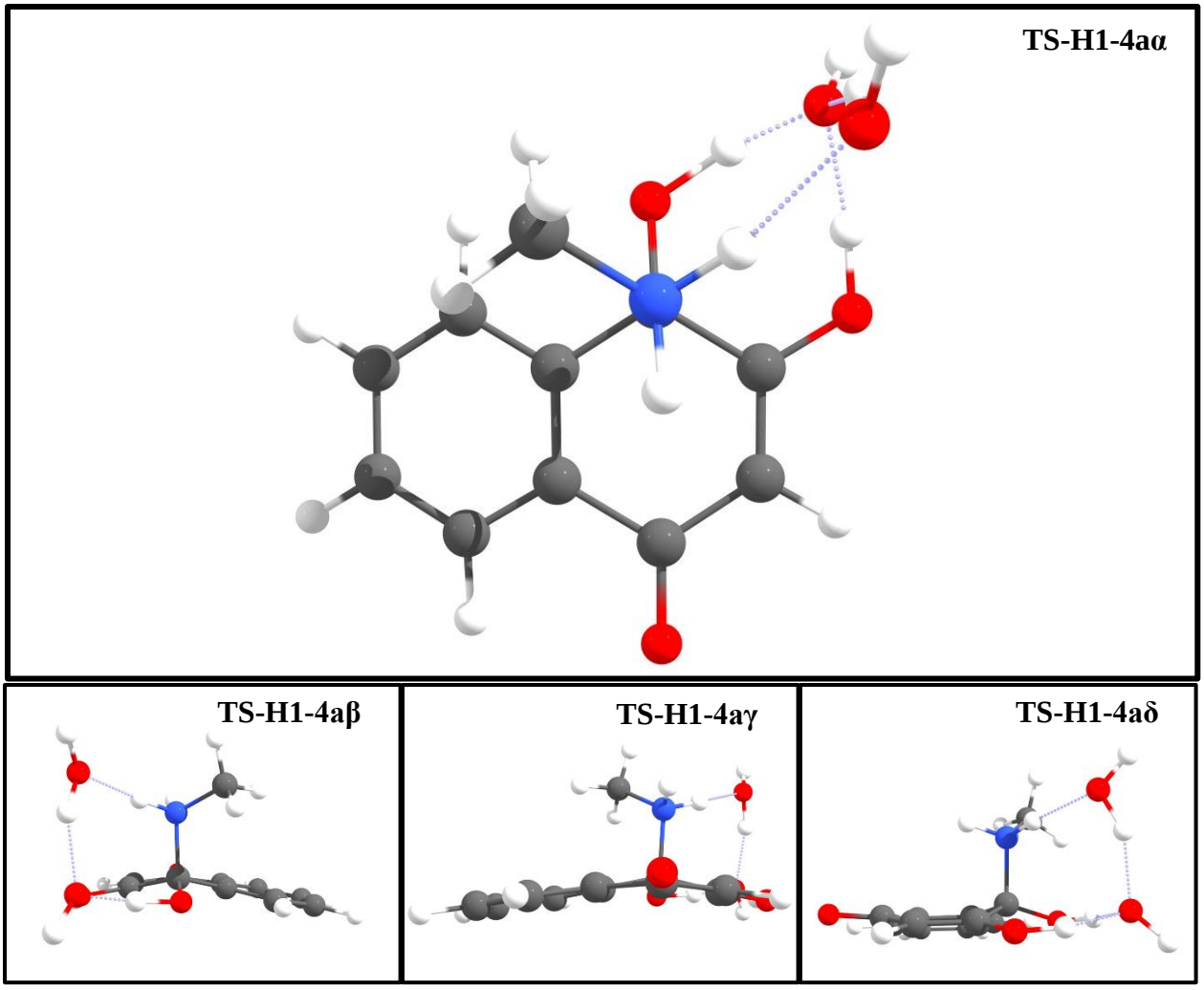


Figure 2.26 Transition state **TS-H1-4a** (early transition state of **TS-H1-4**)

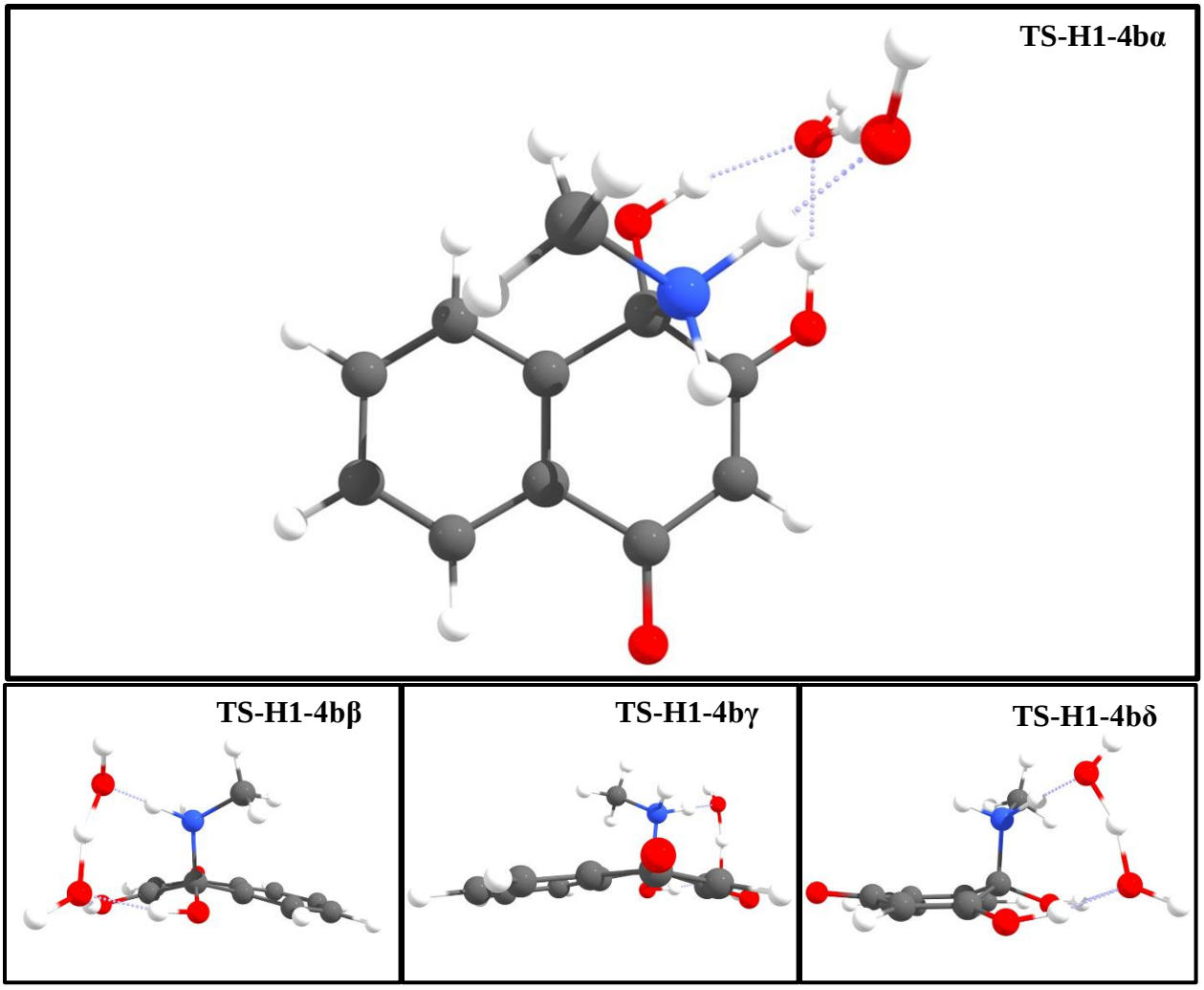


Figure 2.27 Transition state **TS-H1-4b** (late transition state of **TS-H1-4**)

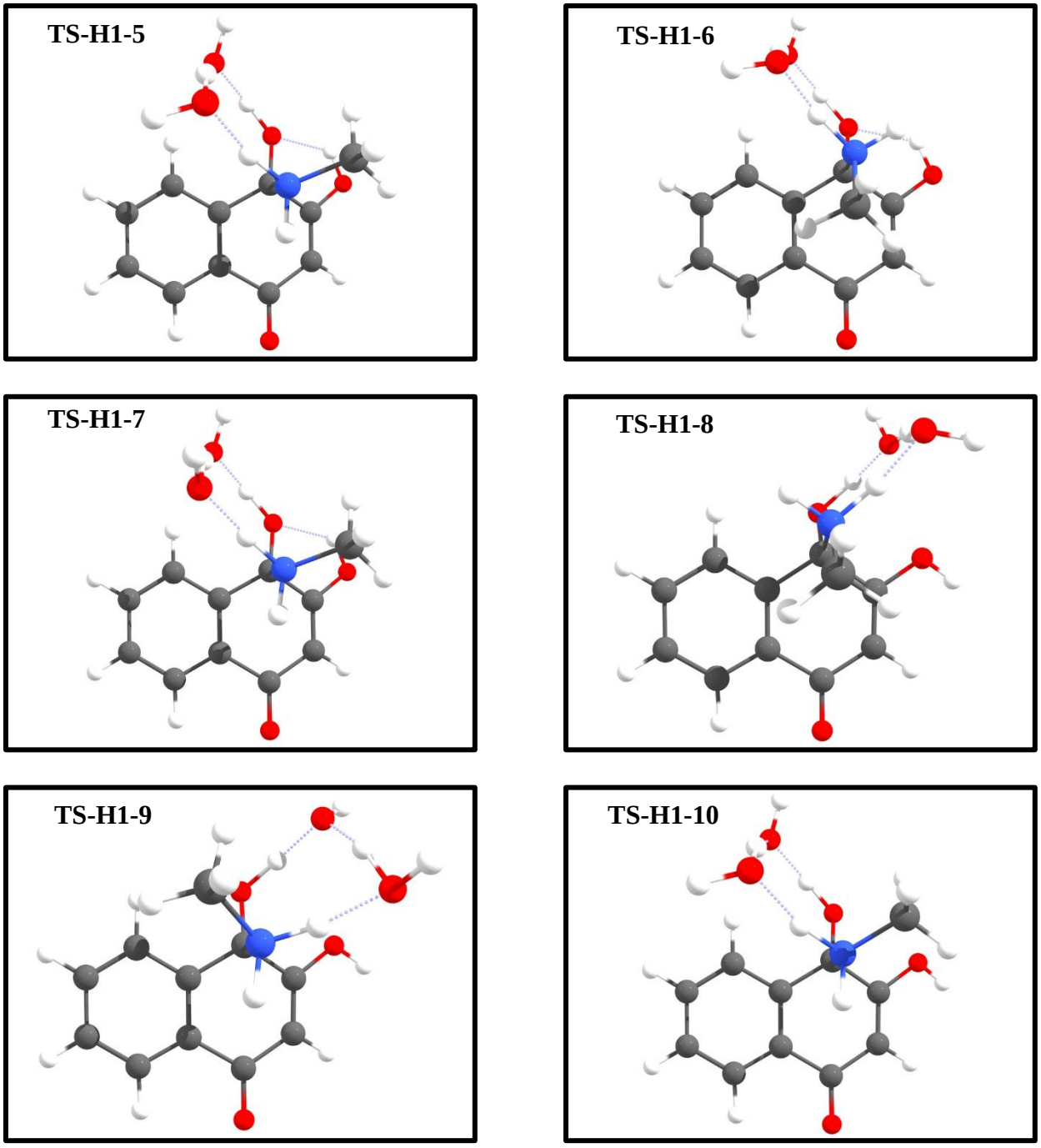


Figure 2.28 Transition states for reaction **R-H1** (energy ranking order 5-10)

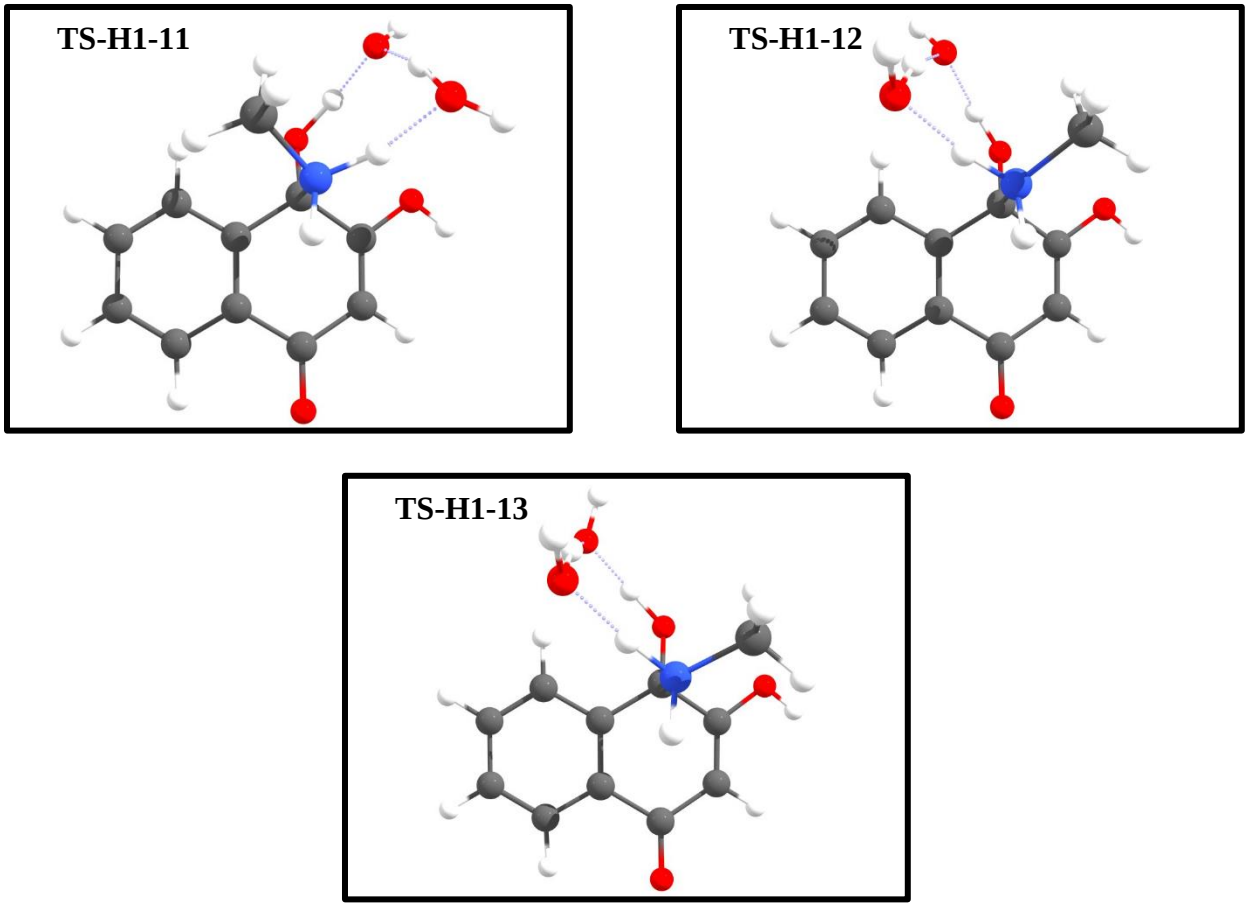


Figure 2.29 Transition states for reaction **R-H1** (energy ranking order 11-13)

2.4.2 1,4-Addition at carbonyl 1 of 2-hydroxy-1,4-naphthoquinone

Thirteen different conformers of the transition state were examined, and only two distinct transition states were identified for the **R-H2** reaction. Some important parameters of the optimized transition states are given in Tables 2.3 and 2.4. **TS-H2-1b** and **TS-H2-1a** were the two lowest energy structures optimized for the transition state of the **R-H2** reaction and are shown in Figures 2.30 and 2.31. The front views of the remaining optimized transition states are depicted in Figure 2.32.

Table 2.3 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-H2**

Saddle point	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-H2-1b	6.84	668*i*
TS-H2-1a	8.39	726*i*
TS-H2-2b	10.06	712*i*
TS-H2-2a	11.28	710*i*

Table 2.4 Selected internuclear distances (Å) for transition state of reaction **R-H2**

Transition State	C_3—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_1—H_x	C_1—O_1
TS-H2-1b	1.482	1.133	1.403	1.146	1.260	1.711	0.984	1.344
TS-H2-1a	1.495	1.049	1.694	0.992	1.657	1.176	1.216	1.305
TS-H2-2b	1.490	1.132	1.402	1.153	1.253	1.702	0.984	1.343
TS-H2-2a	1.503	1.041	1.755	0.991	1.669	1.175	1.216	1.304

As seen in section 2.4.1, the transition states of the **R-H2** reaction also exhibit early and late states. The labeling of these states will remain the same where "a" refers to early transition states while "b" refers to late transition states. As seen in Table 2.3, the late transition state **TS-H2-1b** had the lowest gas-phase barrier height of 6.84 kcal/mol when compared to that of the reactants. The early transition state **TS-H2-1a** had a gas-phase barrier height of 8.39 kcal/mol which is only a 1.55 kcal/mol difference to **TS-H2-1b**. As stated previously, the transition state that represents the higher-energy barrier height must be utilized for each distinct conformation, so for this reaction, the early transition states will be used to represent each distinct conformation. This means that transition state **TS-H2-1a** will represent the energy barrier height

that must be overcome in this reaction. The results shown here suggest that it will not always be the late transition state that will represent each distinction conformation as seen section 2.4.1 and that early transition states can also be used to represent the reaction pathway.

The other distinct transition state, transition state **TS-H2-2a**, in Table 2.3 is higher in energy by 2.89 kcal/mol. The difference between the two distinct transition states is the location of the methyl on the methylamine. By changing the orientation of the methyl, there was a change in the gas-phase barrier height around 3 kcal/mol. For example, transition state **TS-H2-1a**, where the methyl group is pointing forward as seen in Figure 2.31, has a barrier height of 8.39 kcal/mol while transition state **TS-H2-2a**, where the methyl group is pointing toward the side as seen in Figure 2.32 (all other atoms are in similar positions), has a barrier height of 11.28 kcal/mol. In the **R-H2** reaction, there was a greater influence from the methyl position on the energy of the structures when compared to the **R-H1** reaction.

The orientation of the hydroxyl group on the naphthoquinone and the hydrogens on the water molecules were examined, but these factors did not have an influence on the energy as all other conformers optimized to the two distinct conformations presented here. As seen in Table 2.4, the imaginary frequencies that were observed ranges from 668*i* cm^{-1} to 726*i* cm^{-1}.

As shown in Table 2.4, intermolecular distance C_3–N_a has a fairly consistent value around 1.493 Å for all structures. The remaining intermolecular distances are consistent when separated into the early and late transition states. According to Table 2.4, intermolecular distances N_a–H_a, O_w–H_w, O_1–H_x, and C_1–O_1 in early transition states, **TS-H2-1a** and **TS-H2-2a**, have comparatively consistent values around 1.045 Å, 0.991 Å, 1.216 Å and 1.304 Å, respectively, for all the structures. In comparison, the intermolecular distances N_a–H_a, O_w–H_w, O_1–H_x, and C_1–O_1 in the late transition states, **TS-H2-1b** and **TS-H2-2b**, have comparatively

consistent values around 1.132 Å, 1.150 Å, 0.984 Å and 1.344 Å, respectively. As stated in section 2.4.1, the O_1–H_x is longer in the early transition states while C_1–O_1 is longer in the early transition states. The O_1–H_x intermolecular distance depicts how the hydrogen from the second water has not fully transferred to the oxygen on the naphthoquinone ring in the early transition state while the late transition state has already completed this hydrogen transfer. The C_1–O_1 intermolecular distance reflects that the atoms have more double bond character in the early transition state compared to the late transition state. The N_a–H_a and O_w–H_w intermolecular distances for the early transition states are shorter when compared to the late transition states. These distances suggest that the hydrogens from the amine and the first water in the early transition states have not started to transfer when compared to the late transition states. These results are consistent with the model of the early and late transition states presented in section 2.4.1.

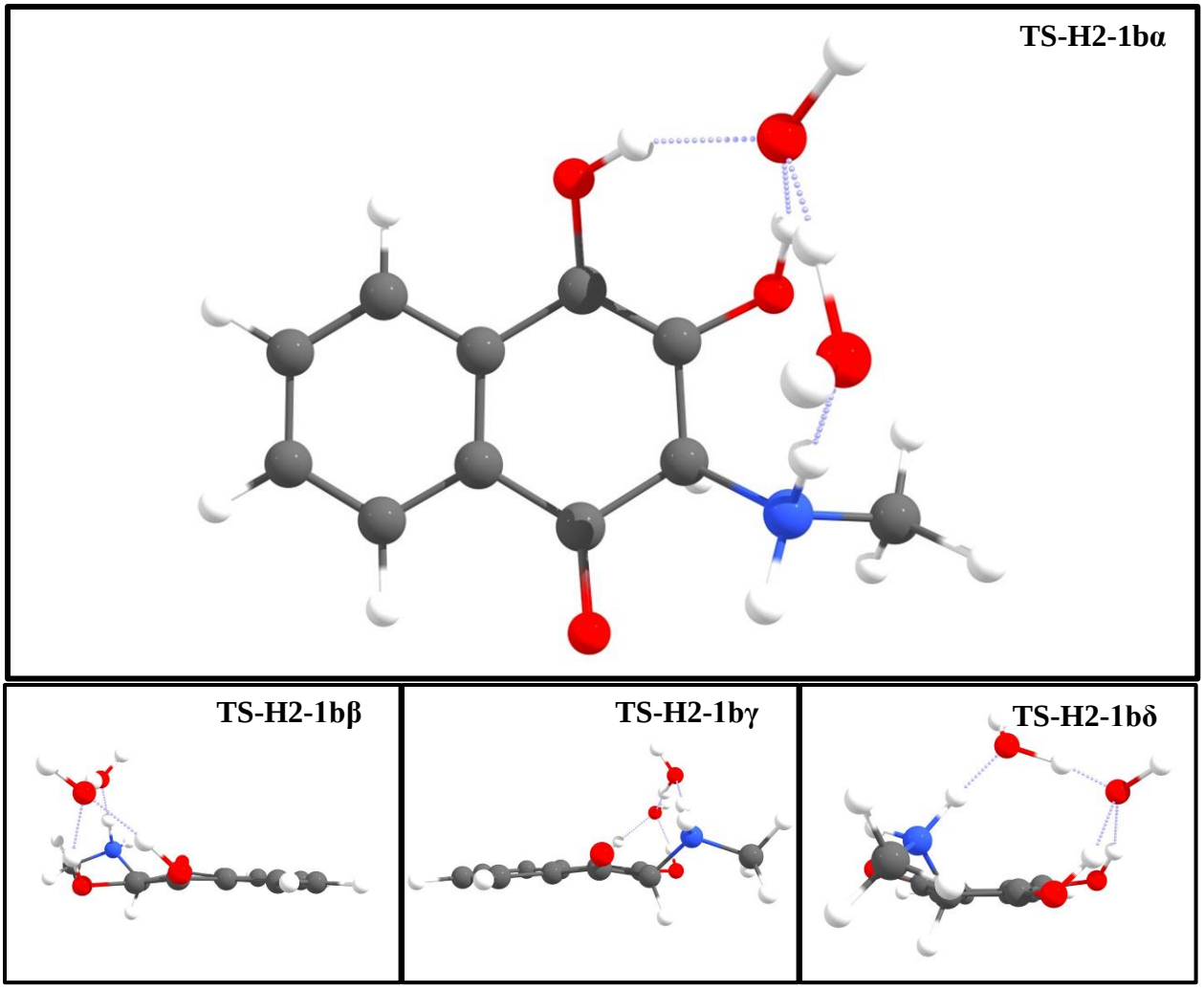


Figure 2.30 Transition state **TS-H2-1b**: Lowest energy structure for transition state of **R-H2** reaction

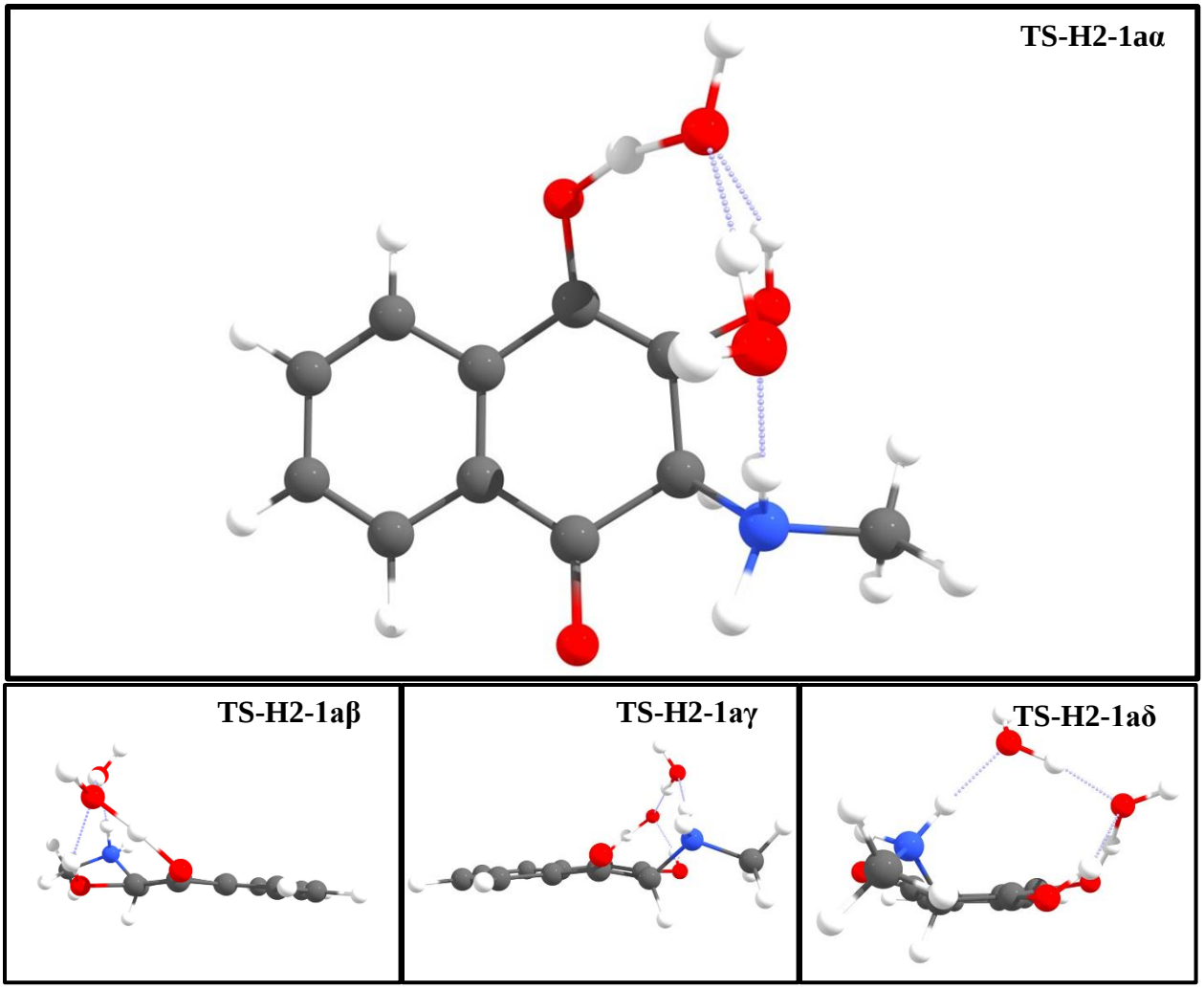


Figure 2.31 Transition state **TS-H1-1a**: Second lowest energy structure for **R-H2** reaction

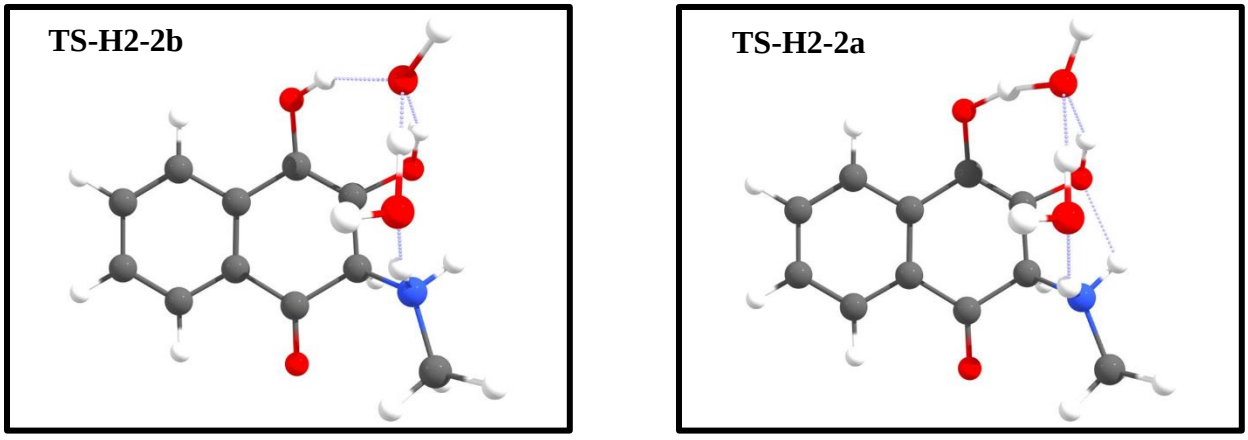


Figure 2.32 Transition states for reaction **R-H2** (energy ranking order 2b-2a)

2.4.3 1,2-Addition at carbonyl 4 of 2-hydroxy-1,4-naphthoquinone

Fourteen different conformers of the transition state were examined, and only ten distinct transition states were identified for the **R-H3** reaction. Some important parameters of the optimized transition states are given in Tables 2.5 and 2.6. **TS-H3-1**, **TS-H3-2**, and **TS-H3-3** were the three lowest energy structures optimized for the transition state of the **R-H3** reaction and are shown in Figures 2.33, 2.34 and 2.35. The front views of the remaining optimized transition states are depicted in Figure 2.36 and 2.37.

Table 2.5 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-H3**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-H3-1	12.03	666*i*
TS-H3-2	12.62	678*i*
TS-H3-3	13.04	676*i*
TS-H3-4	13.43	765*i*
TS-H3-5	13.59	559*i*
TS-H3-6	13.69	514*i*
TS-H3-7	13.98	712*i*
TS-H3-8	18.18	471*i*
TS-H3-9	18.50	511*i*
TS-H3-10	18.85	557*i*

As seen in Table 2.5, the transition state **TS-H3-1** was the lowest gas-phase barrier height of 12.03 kcal/mol when compared to the energy of the reactants. The transition states **TS-H3-2** to **TS-H3-7** only had a gas-phase barrier height difference of less than 2 kcal/mol when

compared to **TS-H3-1**. In comparison, the remaining transition states in Table 2.5, **TS-H3-8** to **TS-H3-10**, are more than 6 kcal/mol higher. As seen in Table 2.6, the imaginary frequencies that were observed ranges from 471*i* cm^{-1} to 765*i* cm^{-1}.

Table 2.6 Selected internuclear distances (Å) for transition state of reaction **R-H3**

Transition State	C_4—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_4—H_x	C_4—O_4
TS-H3-1	1.555	1.097	1.466	1.120	1.282	1.339	1.089	1.345
TS-H3-2	1.565	1.099	1.462	1.126	1.274	1.351	1.081	1.340
TS-H3-3	1.556	1.095	1.470	1.124	1.278	1.344	1.084	1.346
TS-H3-4	1.566	1.099	1.466	1.135	1.259	1.331	1.089	1.339
TS-H3-5	1.548	1.097	1.473	1.128	1.268	1.431	1.045	1.347
TS-H3-6	1.550	1.092	1.484	1.112	1.291	1.385	1.067	1.346
TS-H3-7	1.566	1.098	1.461	1.130	1.268	1.350	1.080	1.341
TS-H3-8	1.556	1.087	1.493	1.109	1.299	1.377	1.071	1.347
TS-H3-9	1.557	1.086	1.498	1.116	1.291	1.383	1.066	1.348
TS-H3-10	1.557	1.086	1.507	1.121	1.277	1.365	1.071	1.346

As shown in Table 2.6, intermolecular distances C_4–N_a, N_a–H_a, O_4–H_x, and C_4–O_4 have fairly consistent values around 1.558 Å, 1.094 Å, 1.074 Å, and 1.3445 Å, respectively. The remaining intermolecular distances shown in Table 2.6 have slight variations that do not show a trend.

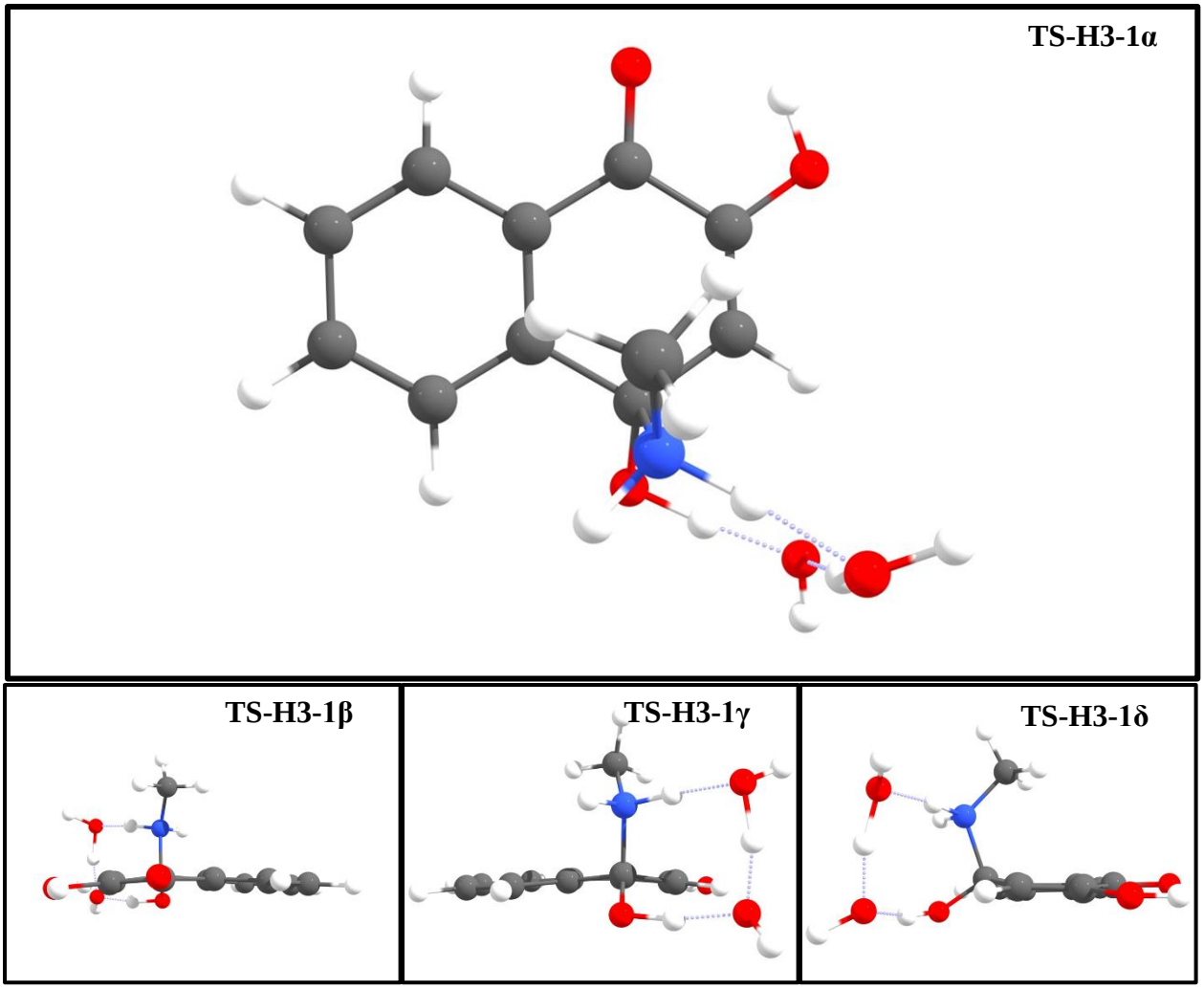


Figure 2.33 Transition state **TS-H3-1**: Lowest energy structure for **R-H3** reaction

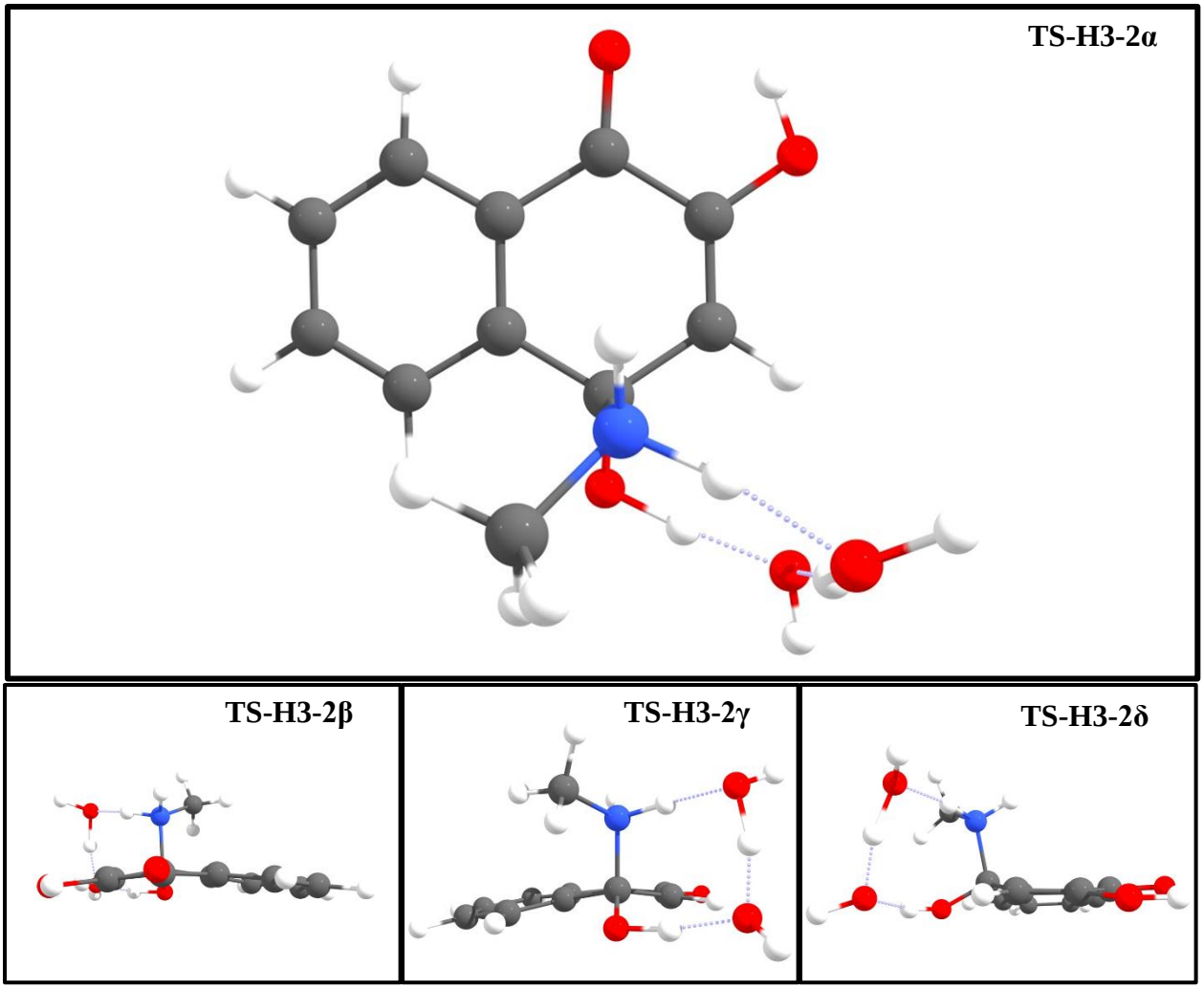


Figure 2.34 Transition state **TS-H3-2**: Second lowest energy structure for **R-H3** reaction

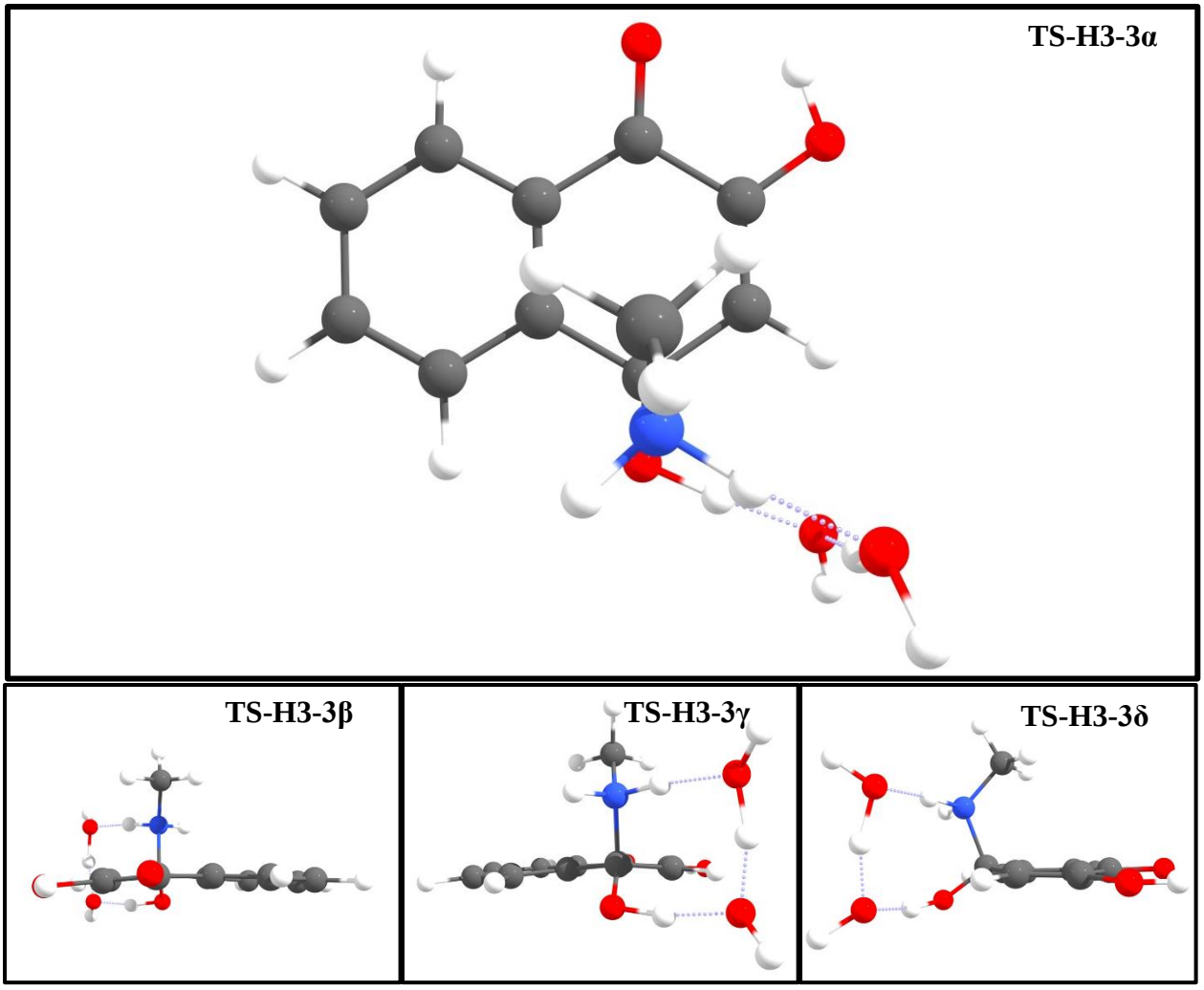


Figure 2.35 Transition state **TS-H3-3**: Third lowest energy structure for **R-H3** reaction

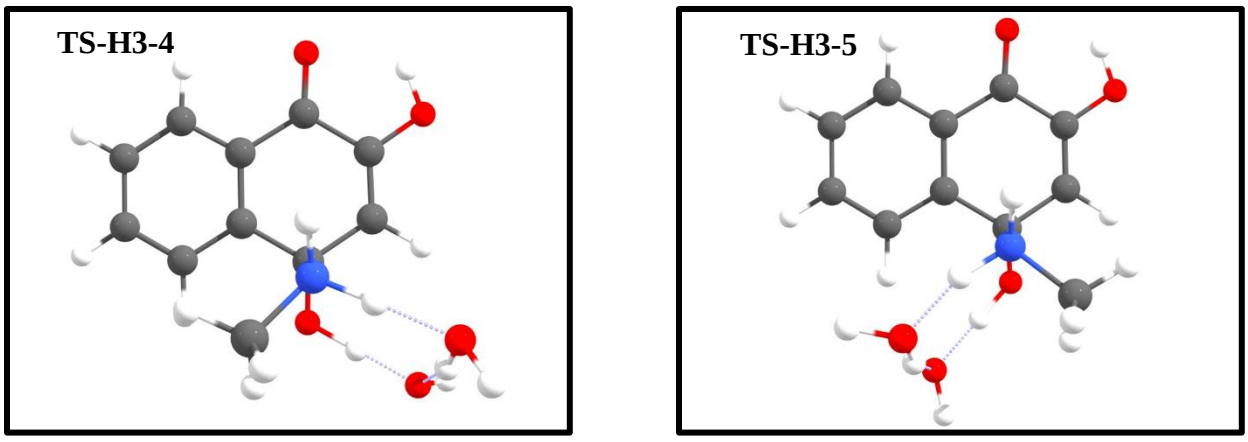


Figure 2.36 Transition states for reaction **R-H3** (energy ranking order 4-5)

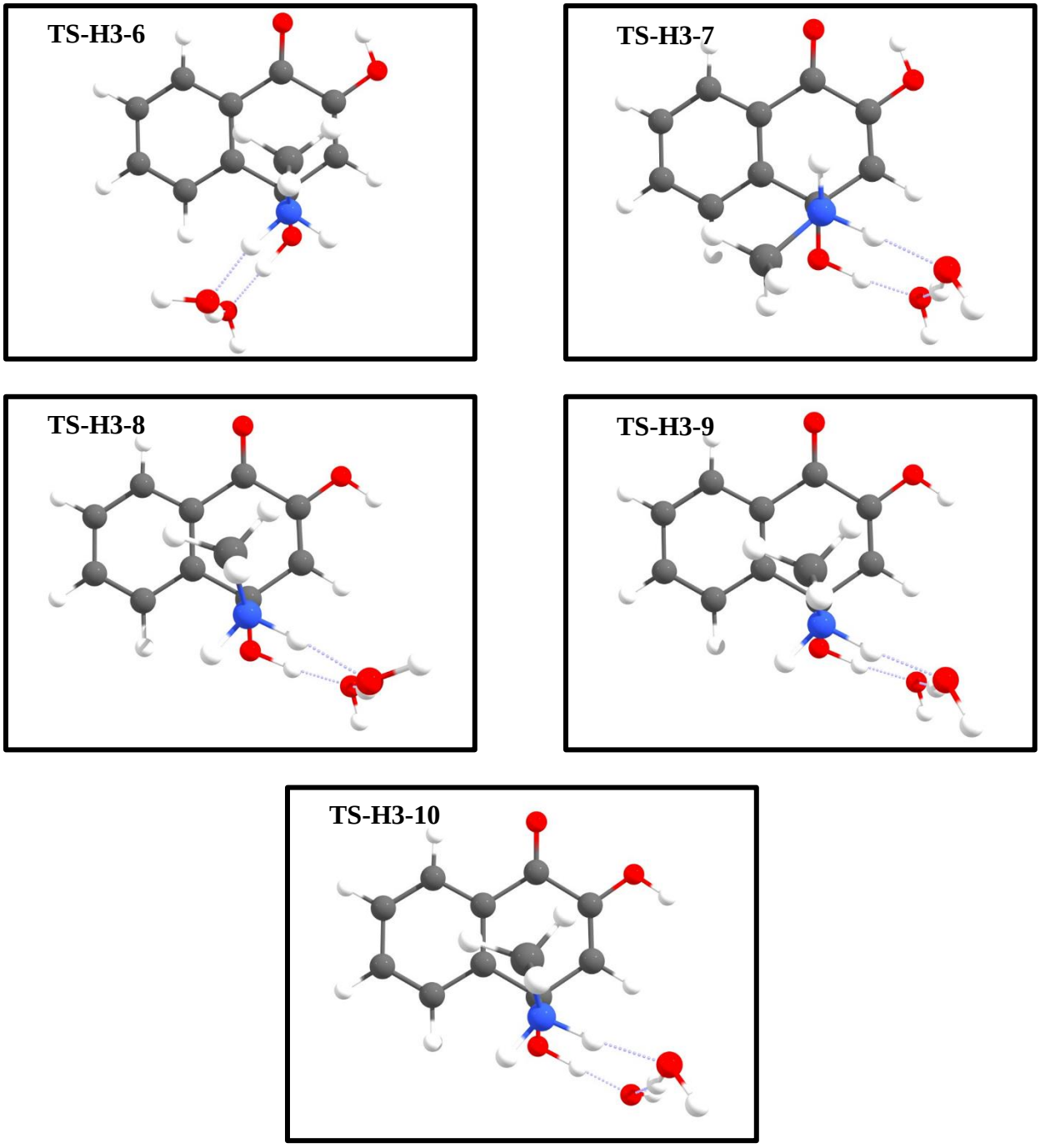


Figure 2.37 Transition states for reaction **R-H3** (energy ranking order 6-10)

2.4.4 1,4-Addition at carbonyl 4 of 2-hydroxy-1,4-naphthoquinone

Thirteen different conformers of the transition state were examined, and only nine distinct transition states were identified for the **R-H4** reaction. Some important parameters of the optimized transition states are given in Tables 2.5 and 2.6. **TS-H4-1**, **TS-H4-2**, **TS-H4-3**, and **TS-H4-4** were the four lowest energy structures optimized for the transition state of the **R-H4** reaction and are shown in Figures 2.38, 2.39, 2.40 and 2.41. The front views of the remaining optimized transition states are depicted in Figure 2.41.

Table 2.7 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-H4**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-H4-1	15.14	1049*i*
TS-H4-2	15.36	1140*i*
TS-H4-3	15.39	1182*i*
TS-H4-4	16.21	870*i*
TS-H4-5	17.24	1196*i*
TS-H4-6	17.32	1249*i*
TS-H4-7	17.58	1334*i*
TS-H4-8	17.70	1346*i*
TS-H4-9	18.26	1152*i*

Table 2.8 Selected internuclear distances (Å) for transition state of reaction **R-H4**

Transition State	C_2—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_4—H_x	C_4—O_4
TS-H4-1	1.488	1.128	1.409	1.149	1.257	1.301	1.115	1.300
TS-H4-2	1.489	1.123	1.409	1.161	1.244	1.281	1.128	1.298
TS-H4-3	1.487	1.135	1.392	1.161	1.237	1.269	1.134	1.298
TS-H4-4	1.523	1.115	1.434	1.127	1.285	1.324	1.103	1.309
TS-H4-5	1.524	1.142	1.380	1.149	1.253	1.257	1.143	1.304
TS-H4-6	1.515	1.145	1.371	1.156	1.239	1.231	1.160	1.301
TS-H4-7	1.522	1.160	1.343	1.168	1.224	1.214	1.172	1.301
TS-H4-8	1.521	1.162	1.346	1.162	1.234	1.224	1.169	1.304
TS-H4-9	1.530	1.120	1.409	1.152	1.249	1.260	1.140	1.302

As seen in Table 2.7, the transition state **TS-H4-1** was the lowest gas-phase barrier height of 15.14 kcal/mol when compared to the energy of the reactants. The transition states **TS-H4-2** to **TS-H4-4** only had a gas-phase barrier height difference of less than 2 kcal/mol when compared to **TS-H4-1**. In comparison, the remaining transition states in Table 2.7, **TS-H3-5** to **TS-H3-9**, are more than 2 kcal/mol higher. Transition state **TS-H4-9** was the highest gas-phase barrier height with 18.26 kcal/mol which is only 3 kcal/mol higher than transition state **TS-H4-1**. As seen in Table 2.8, the imaginary frequencies are within the range of 1049*i* cm^{-1} to 1346*i* cm^{-1}. The only exception is transition state **TS-H4-4** that has an imaginary frequency of 870*i* cm^{-1} and can be considered an outlier.

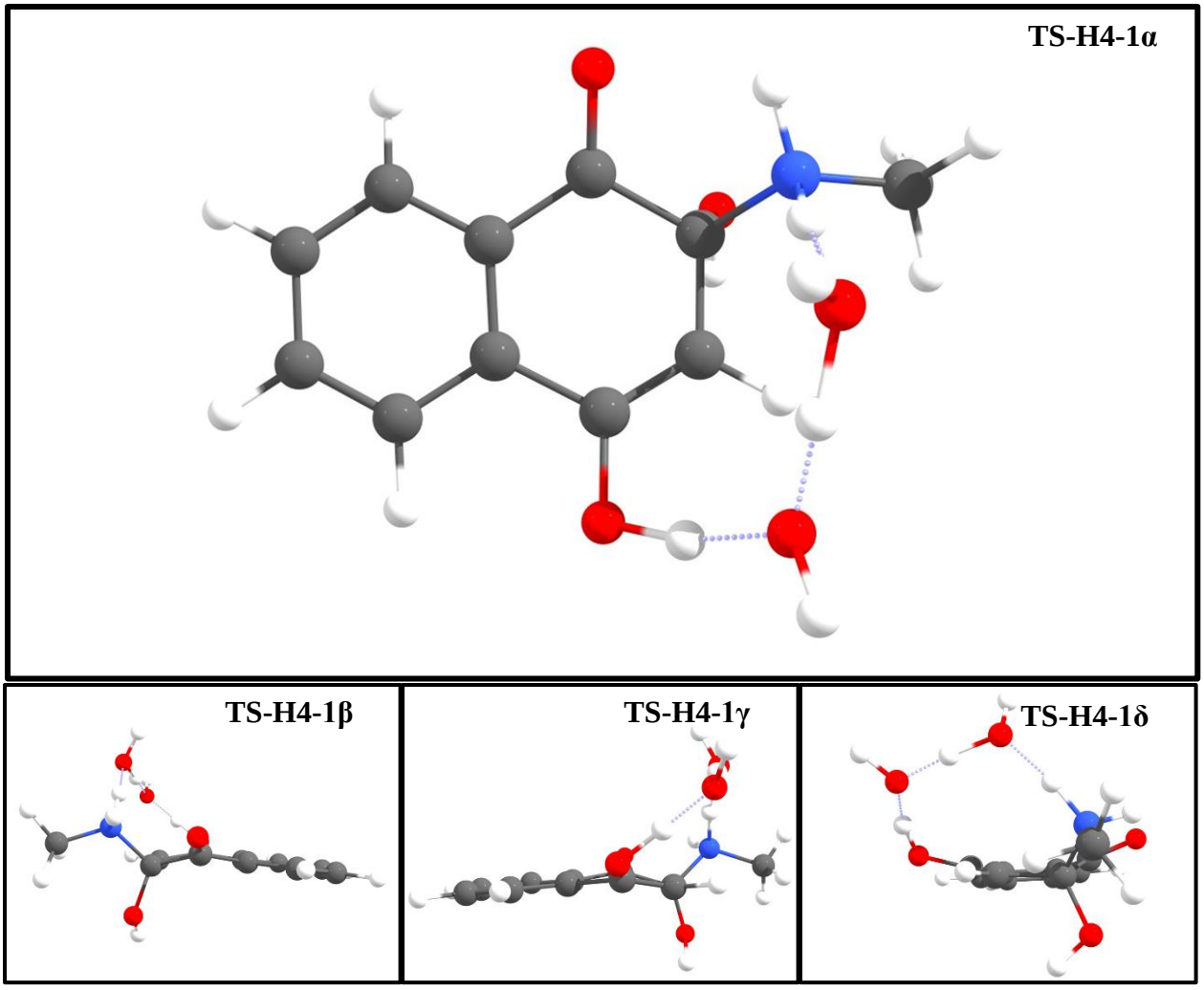


Figure 2.38 Transition state **TS-H4-1**: Lowest energy structure for **R-H4** reaction

As shown in Table 2.8, the only intermolecular distance with a fairly consistent value is C_4–O_4 with a value around 1.302 Å. The only other trend that could be seen is in C_2–N_a which has to be separated into two groups. Transition states **TS-H4-1** to **TS-H4-3** has a fairly consistent value for C_2–N_a at 1.488 Å. In comparison, transition states **TS-H4-4** to **TS-H4-9** has a fairly consistent value for C_2–N_a at 1.523 Å. The C_2–N_a intermolecular distance of the first group is shorter when compared to the second group and might suggest that the lower energy structures have the methylamine forming the bond between the C_2 and N_a earlier. The remaining

intermolecular distances shown in Table 2.8 have slight variations that do not show a trend as some tend to be at a different point in the hydrogen transfer in their optimized states.

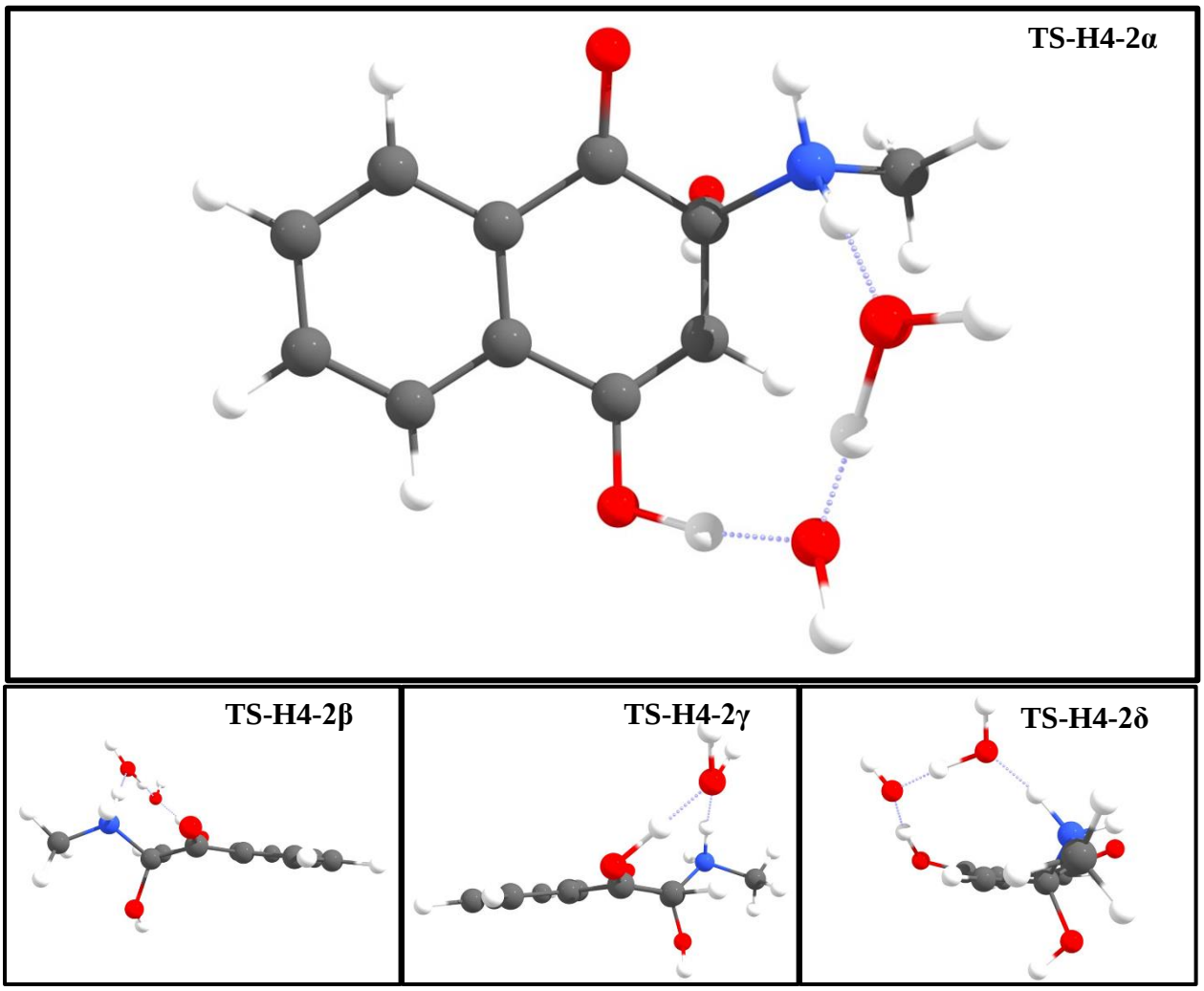


Figure 2.39 Transition state **TS-H4-2**: Second lowest energy structure for **R-H4** reaction

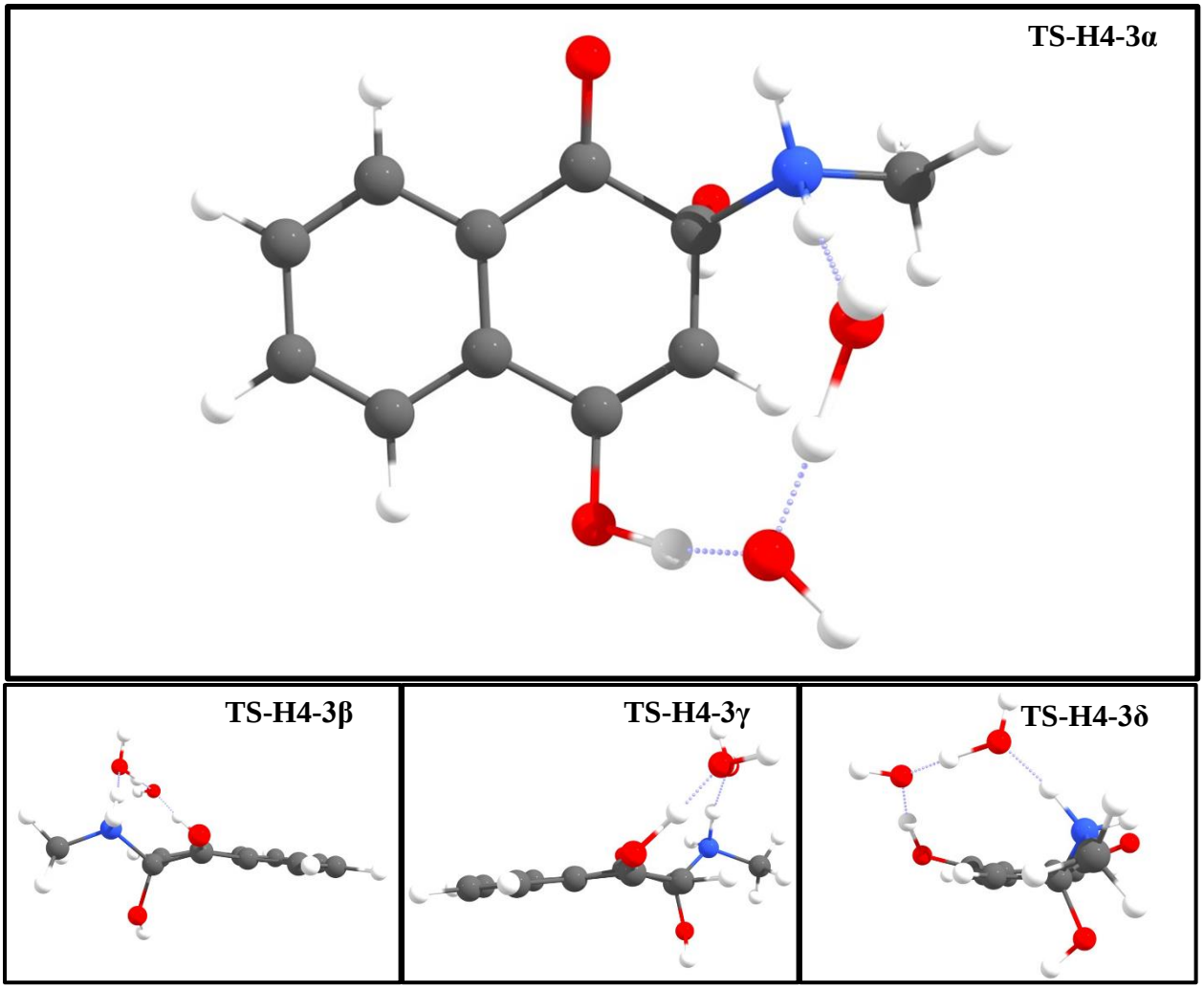


Figure 2.40 Transition state **TS-H4-3**: Third lowest energy structure **R-H4** reaction

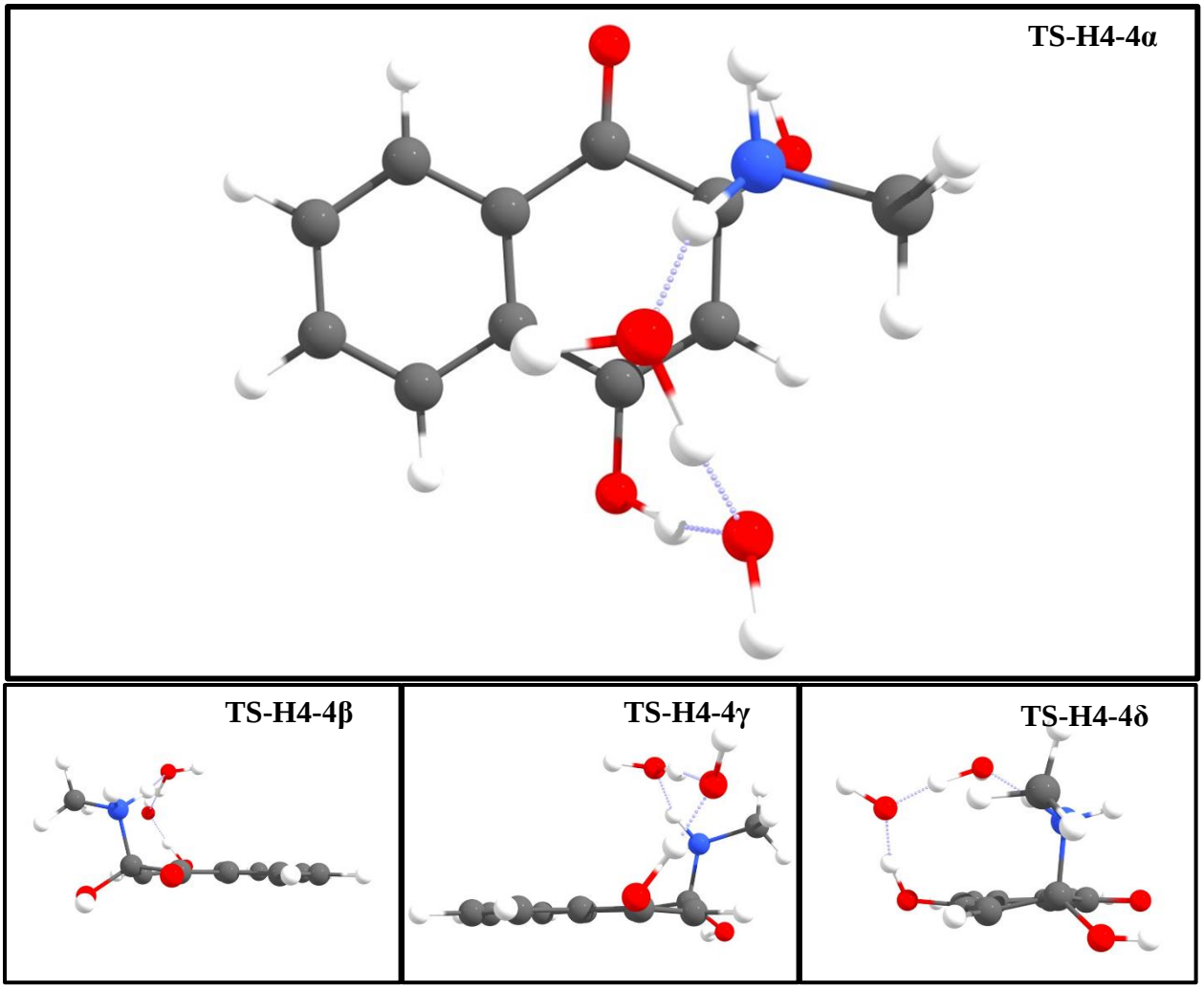


Figure 2.41 Transition state **TS-H4-4**: Fourth lowest energy structure for **R-H4** reaction

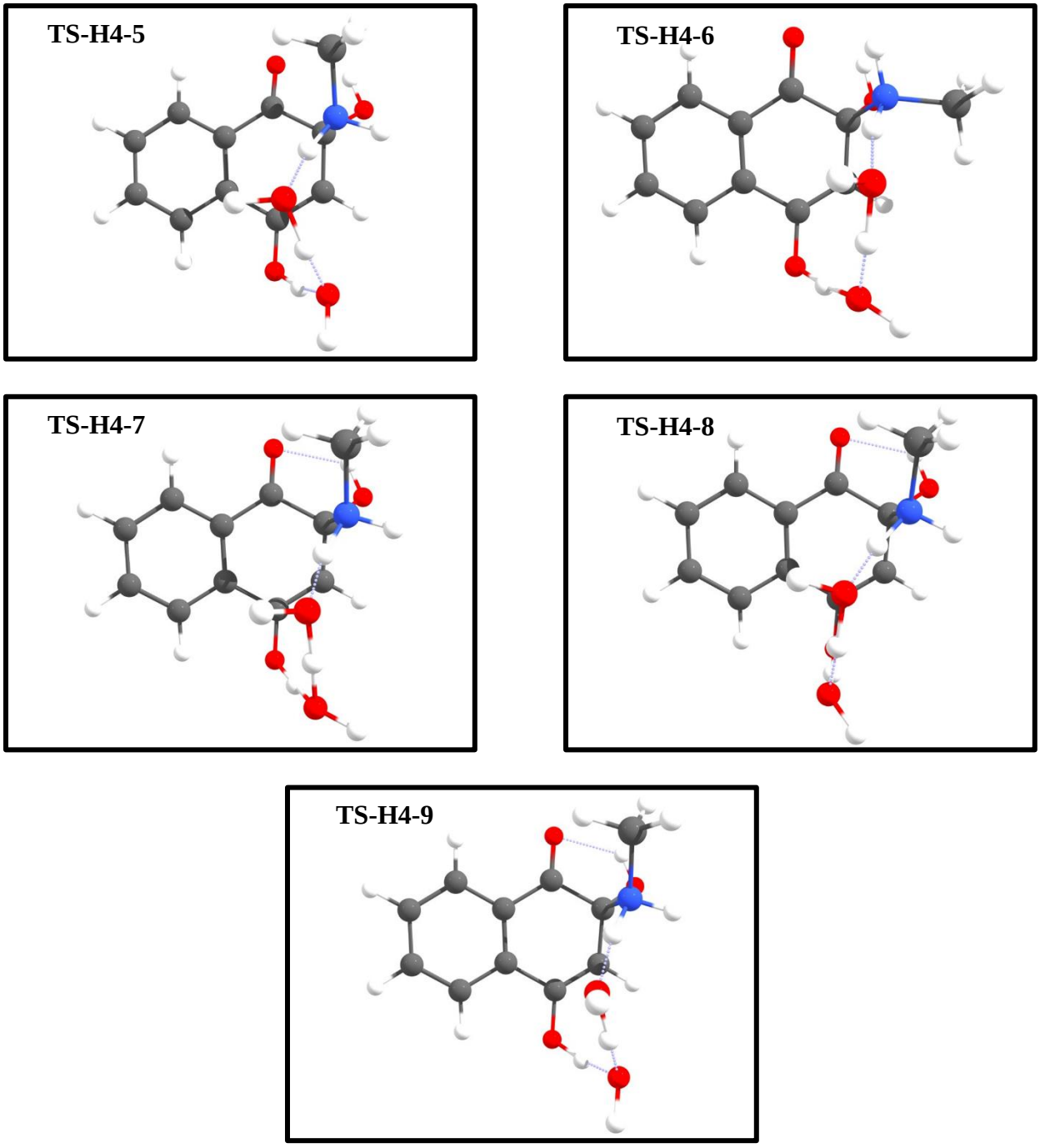


Figure 2.42 Transition states for reaction **R-H4** (energy ranking order 5-9)

2.5 Energy diagram for the reaction between HNQ and methylamine

As stated in section 2.1, each reaction pathway has reactants, reactant complexes, transition states, and products that must be examined to understand the overall reactivity of the naphthoquinone toward the amino group of methylamine. As a result, all the individual stages of the reaction pathway between 2-hydroxy-1,4-naphthoquinone and methylamine has been investigated. Now, it is necessary to consider the important information from each section that examined the individual stages.

The lowest gas-phase barrier height structure of 2-hydroxy-1,4-naphthoquinone and the two water molecules with methylamine as a trimer in section 2.2 were utilized to represent the energy of the reactants. In addition, the energy of the reactants was used as a reference (i.e., having a value of 0.00 kcal/mol), and all other structures have energy values relative to it. Next, the transition states were examined for each possible reaction pathway. The lowest gas-phase barrier heights of the transition states for the **R-H1**, **R-H2**, **R-H3**, and **R-H4** reactions are 4.50 kcal/mol, 8.39 kcal/mol, 12.03 kcal/mol, and 15.14 kcal/mol, respectively. From these values, the **R-H1** reaction, 1,2-addition at carbonyl 1, is the most likely pathway for the reaction to occur. After determining this, one will take the lowest gas-phase barrier height of the products for the **R-H1** reaction and the water dimer calculated in section 2.3 to represent the energy of the products in the overall reaction pathway. The relative energy of the products to the reactants was determined to be 5.71 kcal/mol. Another stage examined in the reaction pathway was the reactant complex. The lowest energy structure for the reactant complexes was determined to be -9.14 kcal/mol relative to the reactants. From this value, the difference between the transition state for the **R-H1** reaction and the reactant complex can be calculated. The relative energy difference is

13.64 kcal/mol and would give a more accurate representation of the barrier height for the reaction occurring in solution. Using this information, the energy diagram of the reaction was constructed and is shown in Figure 2.43.

The product **P-H1-1**, which is represented in Figure 2.43, is 0.15 kcal/mol lower in energy than product **P-H2-1**, 2.67 kcal/mol lower in energy than product **P-H3-1**, and 4.94 kcal/mol lower in energy than product **P-H4-1**. These energy values suggest that the product **P-H1-1** is the lowest energy product and is the most stable product conformation.

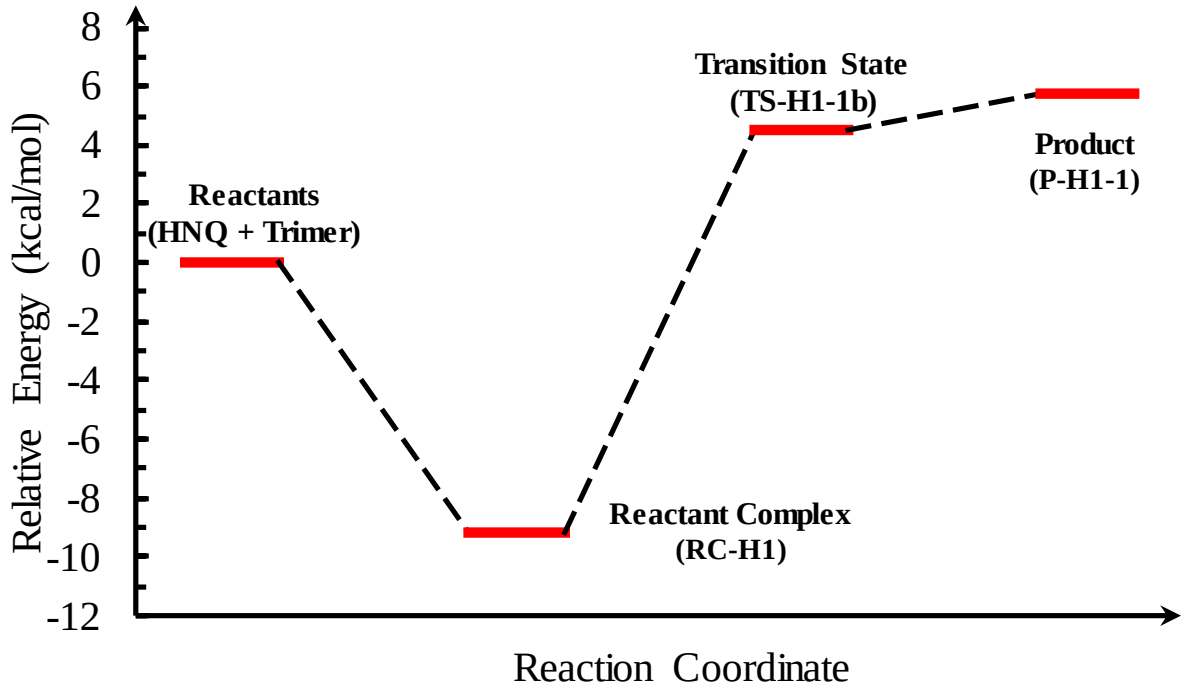


Figure 2.43 Energy diagram for the reaction between 2-hydroxy-1,4-naphthoquinone and methylamine in the presence of two water molecules

CHAPTER 3

REACTIVITY OF 1,4-NAPHTHOQUINONE

3.1 Introduction

The second reaction investigated was the first step of the reaction between 1,4-napthoquinone or *para*-naphthoquinone (PNQ) and methylamine, CH_3NH_2. Figure 3.1 depicts the numbering of the carbon atoms on PNQ throughout this study. For the reaction between PNQ and CH_3NH_2, there are only two different product isomers that can be formed since there is only one unique carbonyl positions and two possible reactions for each carbonyl position. Therefore, the possible reactions are a 1,2-addition at the carbonyl and a 1,4-addition at the carbonyl. Figure 3.2 depicts a general scheme for the possible product isomers that can be formed from the reaction of 1,4-naphthoquinone and CH_3NH_2. All the possible reactions studied for the reaction of PNQ and CH_3NH_2, namely 1,2-addition and 1,4-addition are shown in Figures 3.3 and 3.4 respectively. For each reaction pathway, there are reactants, reactant complexes, transition states, and products that must be examined to understand the overall reactivity of the naphthoquinone toward an amino group. Each of the reactions are labeled **R-Px** where R stands for reaction, P stands for PNQ, and x=1-2 stands for each possible reaction path. Similarly, the two products are labeled $\mathbf{P_{1}\text{-}P2_{x}}$ where the P_1 stands for product and P_2 stands for PNQ.

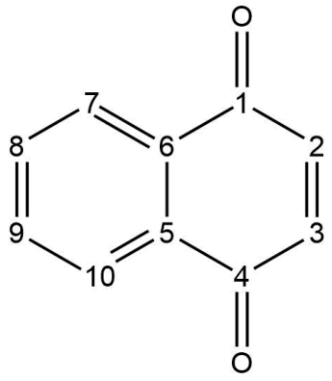


Figure 3.1 Carbon centers numbering of 1,4-naphthoquinone

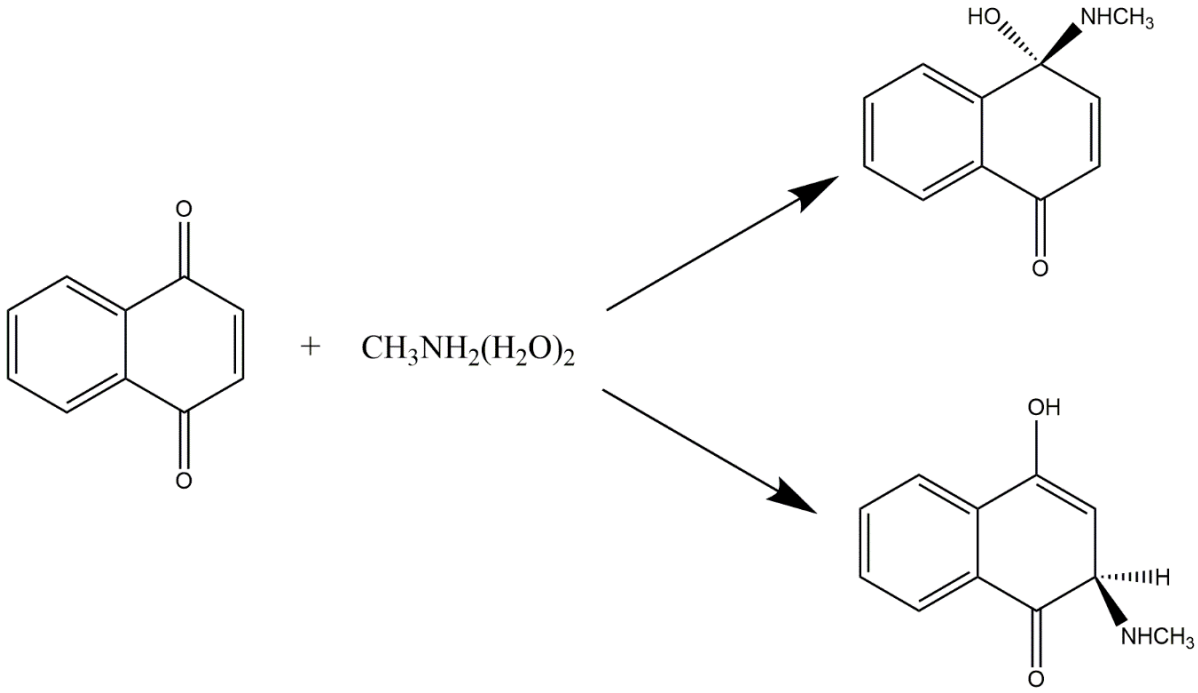
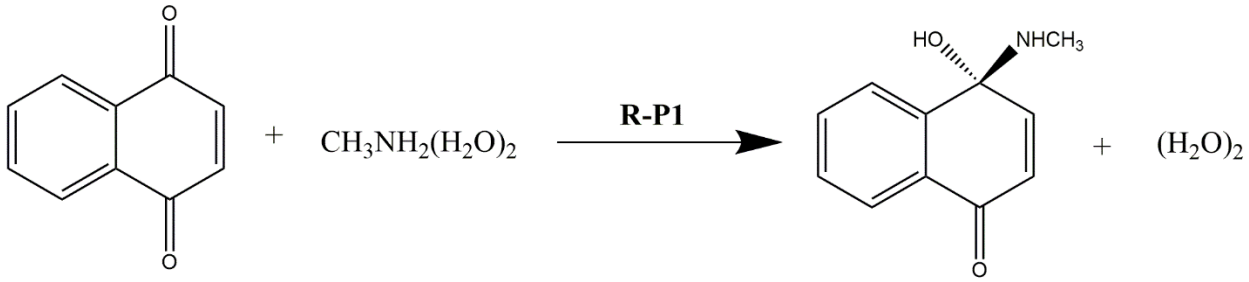
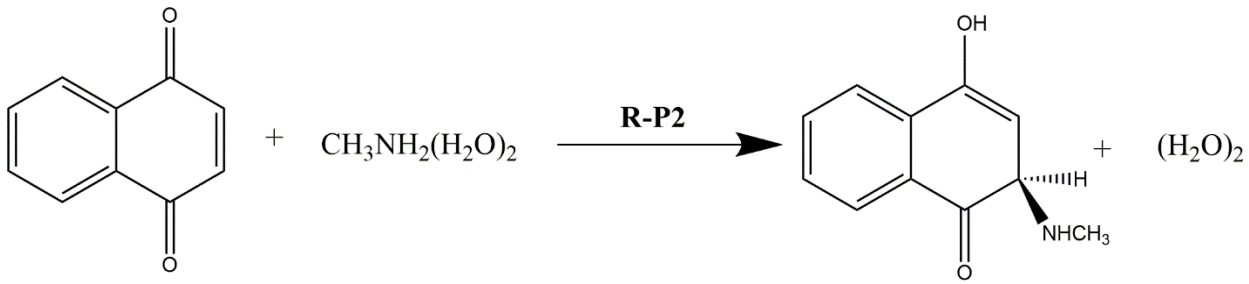


Figure 3.2 Possible reaction pathways for 1,4-naphthoquinone and CH_3NH_2



(P-P1)

Figure 3.3 1,2-Addition between 1,4-naphthoquinone and CH_3NH_2 at the carbonyl



(P-P2)

Figure 3.4 1,4-Addition between 1,4-naphthoquinone and CH_3NH_2 at the carbonyl

3.2 Structure and properties of the reactant state (1,4-naphthoquinone)

3.2.1 1,4-Naphthoquinone as a reactant

As stated previously in section 2.2.1, there must be a point of reference to compare the energy of each structure with that of another structure. Therefore, each stage of reactions in this study must have a reference energy value to compare to which, for this study, will be the energy values of the reactants. The first stage of the reactants will always be the naphthoquinones of interest, and for Chapter 3, this reactant is 1,4-naphthoquinone. 1,4-naphthoquinone only has one

structure that was modeled and optimized. The reactant for 1,4-naphthoquinone is labeled **RE-Px** where RE stands for reactant state, P stands for PNQ, and x is a number to specify a different conformation. Since there is only one structure, x will only be 1. The optimized structure of 1,4-naphthoquinone is shown in Figure 3.5.

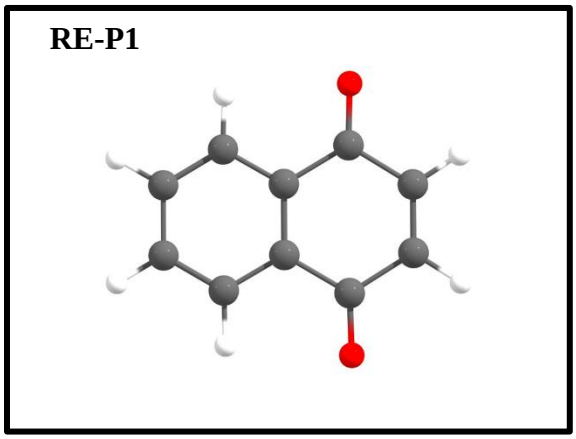


Figure 3.5 **RE-P1**: Optimized structure of 1,4-naphthoquinone

In addition to using the optimized structure of 1,4-naphthoquinone, the energy of the $CH_3HN_2(H_2O)_2$ trimer calculated in section 2.2.2 will be utilized as part of the reactant energy for Chapter 3. It should be noted that all structures in this chapter will be relative to 1,4-naphthoquinone and the $CH_3HN_2(H_2O)_2$ trimer unless stated otherwise.

3.2.2 Reactant complexes

Once again, there is the possibility of considering the complex including all the reactants as the reference energy. For this chapter, the two water molecules, methylamine, and a 1,4-naphthoquinone would form a tetramer. Overall, 26 different possible arrangements of the 1,4-

naphthoquinone tetramer were investigated with only 14 unique optimized conformations found. The lowest energy tetramer was determined and depicted in Figure 3.6. Other interesting tetramers are shown in Figure 3.7 and give a good idea of how the molecules within the tetramer likes to orient. Each of these calculations took anywhere from three to eleven days of computation on one processor to determine an optimized structure. The reactant complexes for PNQ are labeled **RC-Px** where RC stands for reactant complex, P stands for PNQ, and x is a number to specify a different conformation. The reactant complexes are labeled from lowest energy to greatest energy, but not all structures are shown here. Only some interesting tetramers are shown in Figure 3.7, so there will be gaps in the labeling of the tetramers. The remaining tetramers' structures can be found in the appendix.

For the tetramer complex, **RC-P1** was determined to be the most stable structure of the tetramer complex. When compared to 1,4-naphthoquinone and the $CH_3HN_2(H_2O)_2$ trimer complex of the reactants, **RC-P1** has a relative energy of -6.19 kcal/mol. The relative energies of **RC-P2**, **RC-P3 RC-P6**, **RC-P8**, **RC-P9**, and **RC-P12** in Figure 3.7 with respect to **RC-P1** are 1.10 kcal/mol, 1.16 kcal/mol, 1.29 kcal/mol, 1.54 kcal/mol, 2.04 kcal/mol, and 3.71 kcal/mol, respectively.

By comparing the optimized orientations and their respective energies, there seems to be a similar trend to the complexes from section 2.2.3 with how the reactants orient themselves. The energy of the complex is generally lower when the two water molecules and methylamine are interacting with one another. This supports the previous observation that the two water molecules and methylamine form a trimer more readily than interacting individually with the naphthoquinone. The only interesting one is RC-P12 that has a higher energy despite the two water molecules and methylamine being in a trimer. This might be due to the hydrogen on the

1,4-naphthoquinone interacting more favorably with the water molecules than the methylamine. Therefore, the orientations with water closer to the hydrogen on the naphthoquinone seem to be lower in energy.

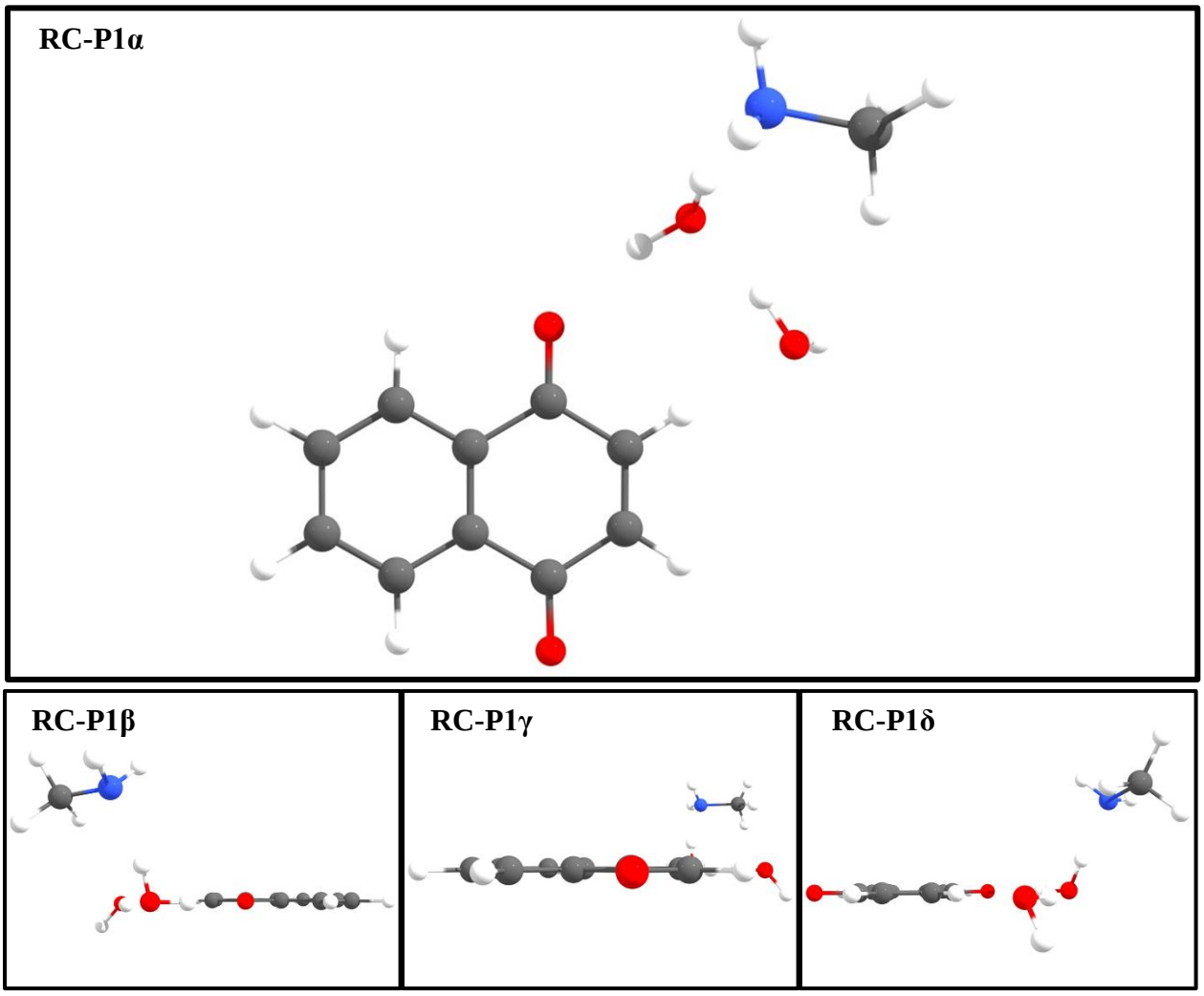


Figure 3.6 Optimized orientation of most stable tetramer complex (1,4-naphthoquinone, methylamine, and two water molecules)

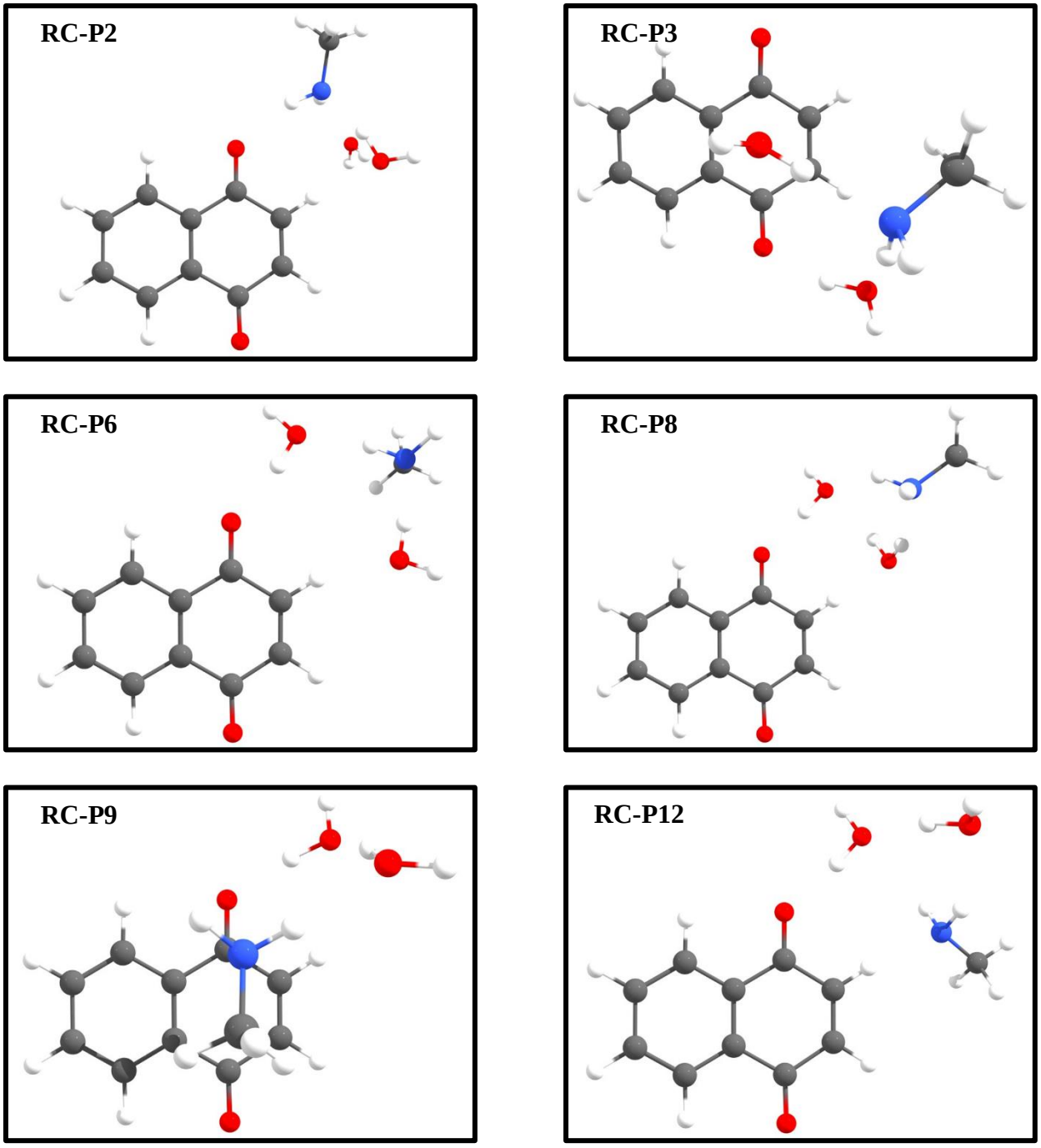


Figure 3.7 Optimized orientations of other tetramer complexes (1,4-naphthoquinone, methylamine, and two water molecules)

3.3 Structure and properties of the product state

The next stage of the reaction between 1,4-naphthoquinone and methylamine depicted in Figure 3.2 is finding the most stable structures of the reaction products. A detailed conformation analysis was carried out for the products in Figure 3.2 where there are 24 possible product conformers based on the two possible reactions. There is a combination of 12 possible orientations for the 1,2-additions and 12 possible orientations for the 1,4-addition. Each product will have a different IUPAC name, but the factors examined will be the same. The factors examined in these possible conformers are the orientation of the OH functional group, formed from the single H atom addition, and the methyl and hydrogen orientations on the binding methylamine. The bound methylamine has a single bond which allows for rotation around the C–N bond, and this rotation was also examined. The calculation time for the optimized geometry of a product conformation is around one to two days. From the 24 possible conformers, 21 distinct product conformations were optimized. Figures 3.8 and 3.9 represent the four lowest energy products from the **R-P1** and **R-P2** reactions, respectively. As stated previously in section 3.1**, $\mathbf{P_1}$-$\mathbf{P_2x_1}$-$\mathbf{x_2}$** where P_1 stands for product, P_2 stands for PNQ, x_1=1-2 stands for each possible reaction path mentioned in section 2.1, and x_2 stands for a distinct conformation. The energy of the dimer of the two water molecules calculated in section 2.3.2 will be utilized with the products calculated in this section to determine the overall energy of the products.

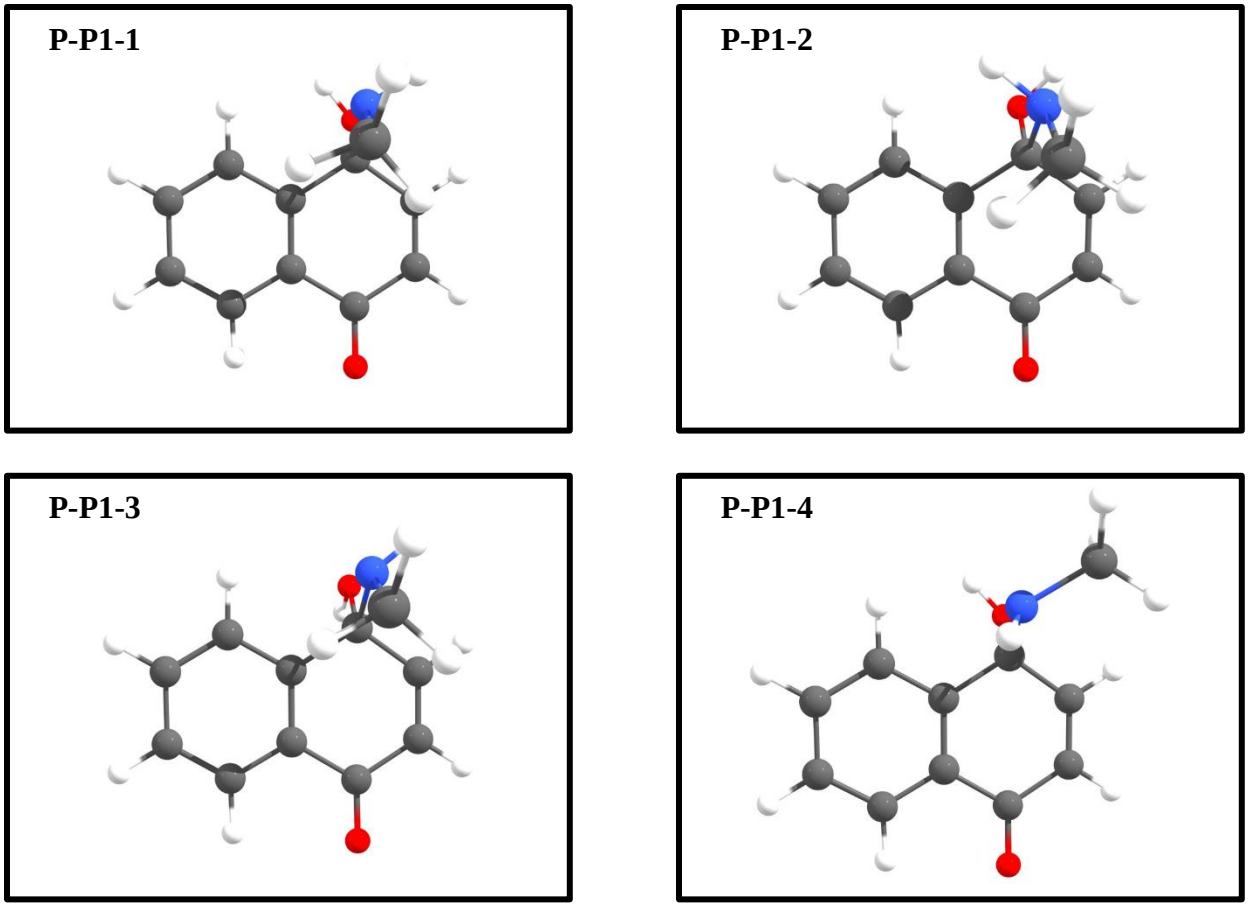


Figure 3.8 **P-P1-1**, **P-P1-2**, **P-P1-3**, and **P-P1-4**: Four lowest energy structures for the product of **R-P1** reaction

Among the four product conformations in Figure 3.8, **P-P1-1** was determined to be the most stable structure for the product of the **R-P1** reaction. The relative energies of **P-P1-2**, **P-P1-3**, and **P-P1-4** with respect to **P-P1-1** are 0.44 kcal/mol, 0.96 kcal/mol, and 0.98 kcal/mol, respectively. For the products of **R-P1**, 10 conformations were optimized, and the least stable conformation has a relative energy of 2.70 kcal/mol. With these low relative energy differences, all of the product conformations could occur, and **P-P1-1** is only the most likely to occur.

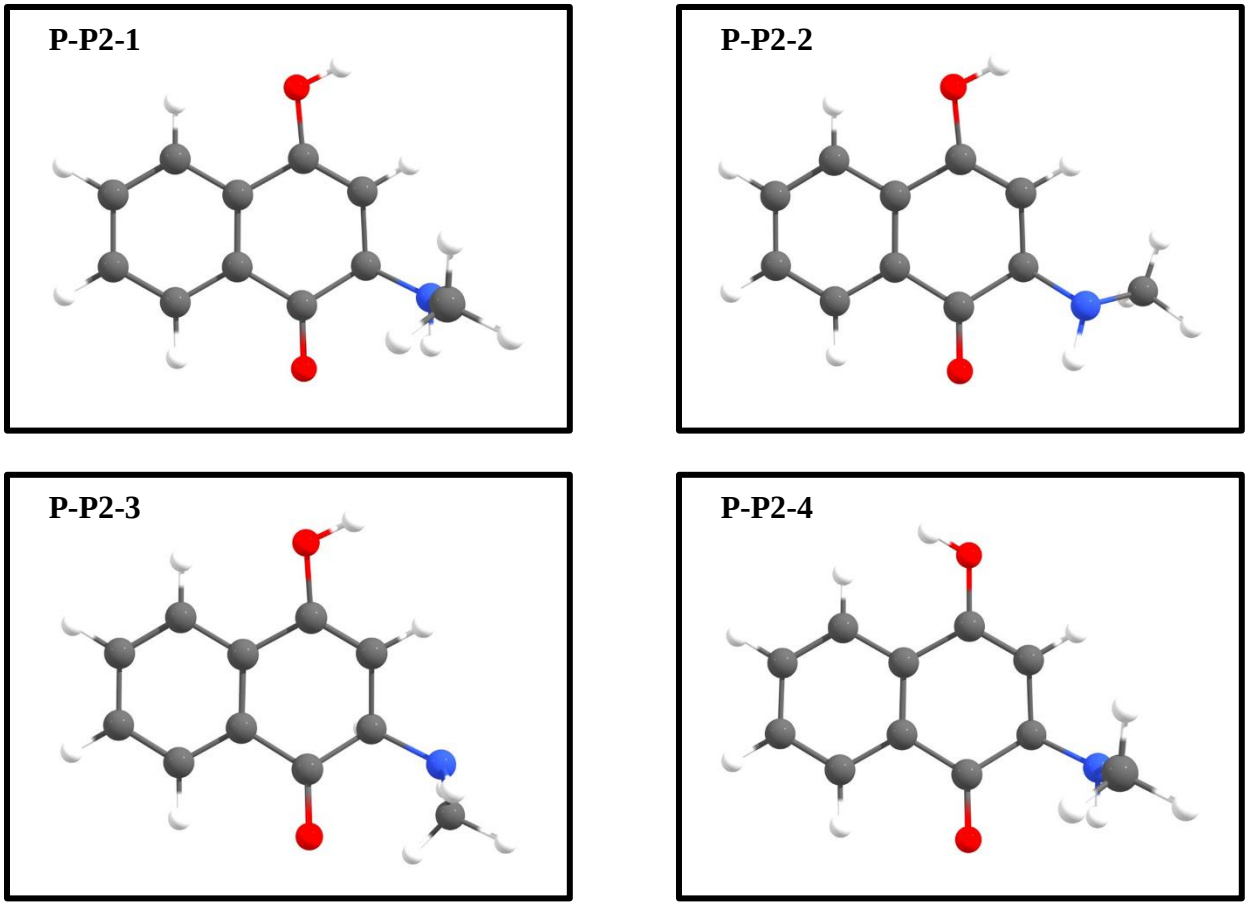


Figure 3.9 **P-P2-1**, **P-P2-2**, **P-P2-3**, and **P-P2-4**: Four lowest energy structures for the product of **R-P2** reaction

Among the four product conformations in Figure 3.9, **P-P2-1** was determined to be the most stable structure for the product of the **R-P2** reaction. The relative energies of **P-P2-2**, **P-P2-3**, and **P-P2-4** with respect to **P-P2-1** are 0.93 kcal/mol, 1,64 kcal/mol, and 2.89 kcal/mol, respectively. For the products of **R-H2**, 11 conformations were optimized, and the least stable conformation has a relative energy of 6.81 kcal/mol compared to the lowest-energy conformation.

3.4 Analysis of transition states

As stated previously, the transition state is the most important stage of the reaction pathway because it determines the energy barrier that must be overcome for the reaction to occur. Therefore, it is necessary to determine the most likely transition state for each possible reaction pathways so that one can determine which reaction is most likely to occur. As stated previously, there will be a focus on the first step of the hydrogen transfer from the nucleophile, methylamine, to the carbonyl group of 1,4-naphthoquinone as the transition state. To study this transition state, the model described in section 2.4 will be utilized to facilitate the hydrogen transfer.

An analysis was carried out for the transition states of 1,2-addition and 1,4-addition. The important factors examined in each transition state in this section are the methyl position on the amine, the location of the hydrogen transfer through the two water molecules, and the position of the hydrogens on the two water molecules. There was a total of 18 transition states examined, and only 12 distinct transition states were obtained. Overall, the calculation times for the optimized geometry of a transition state ranges from two to four days. As for the naming of the structures presented in this study, **TS-Px_1-x_2** where TS stands for transition state, P stands for PNQ, x_1=1-2 stands for each possible reaction path mentioned in section 3.1, and x_2 stands for a different conformation in that possible reaction path.

3.4.1 1,2-Addition of 1,4-naphthoquinone

Ten different conformers of the transition state were examined, and only seven distinct transition states were identified for the **R-P1** reaction. A summary of some important parameters of the transition states are given in Tables 3.1 and 3.2. Once again, the symbols $V^{\ddagger}$ and $\omega^{\ddagger}$ are gas-phase barrier height in kcal/mol and imaginary frequency in cm^{-1}, respectively. The gas-phase barrier height in the tables of this section are relative to energy of the individual naphthoquinone and $CH_3HN_2(H_2O)_2$ trimer energy values. For Table 3.2, the intermolecular distances presented in the table are in angstroms (Å).

Table 3.1 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-P1**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-P1-1	8.87	592*i*
TS-P1-2	9.28	612*i*
TS-P1-3	9.53	673*i*
TS-P1-4	10.07	690*i*
TS-P1-5	10.22	653*i*
TS-P1-6	11.02	581*i*
TS-P1-7	11.06	614*i*

Table 3.2 Selected internuclear distances (Å) for transition state of reaction **R-P1**

Transition State	C_1—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_1—H_x	C_1—O_1
TS-P1-1	1.551	1.093	1.475	1.116	1.289	1.352	1.082	1.345
TS-P1-2	1.560	1.096	1.471	1.122	1.280	1.361	1.077	1.340
TS-P1-3	1.551	1.093	1.483	1.124	1.272	1.336	1.086	1.344
TS-P1-4	1.562	1.096	1.475	1.130	1.264	1.345	1.081	1.339
TS-P1-5	1.562	1.095	1.469	1.126	1.275	1.361	1.075	1.340
TS-P1-6	1.546	1.103	1.459	1.120	1.279	1.390	1.061	1.344
TS-P1-7	1.547	1.100	1.461	1.112	1.290	1.353	1.082	1.344

TS-P1-1, **TS-P1-2**, and **TS-P1-3** were the three lowest energy structures optimized for the transition state of the **R-P1** reaction and are shown in Figures 3.10, 3.11, and 3.12. The front views of the remaining optimized transition states are depicted in Figure 3.13.

As seen in Table 3.1, the transition state **TS-P1-1** was the lowest gas-phase barrier height of 8.87 kcal/mol when compared to that of the reactants. The next two transition states **TS-P1-2** and **TS-P1-3** had gas-phase barrier heights of 9.28 kcal/mol and 9.53 kcal/mol which only have a less than 1 kcal/mol difference to the **TS-P1-1**. The remaining transition states in Table 3.1 are not much higher in energy with transition state **TS-P1-7** having the highest gas-phase barrier at 11.06 kcal/mol. This is still less than a 3 kcal/mol difference between all structures. As seen in Table 3.1, the imaginary frequencies that were observed ranges from 581*i* cm^{-1} to 690*i* cm^{-1}.

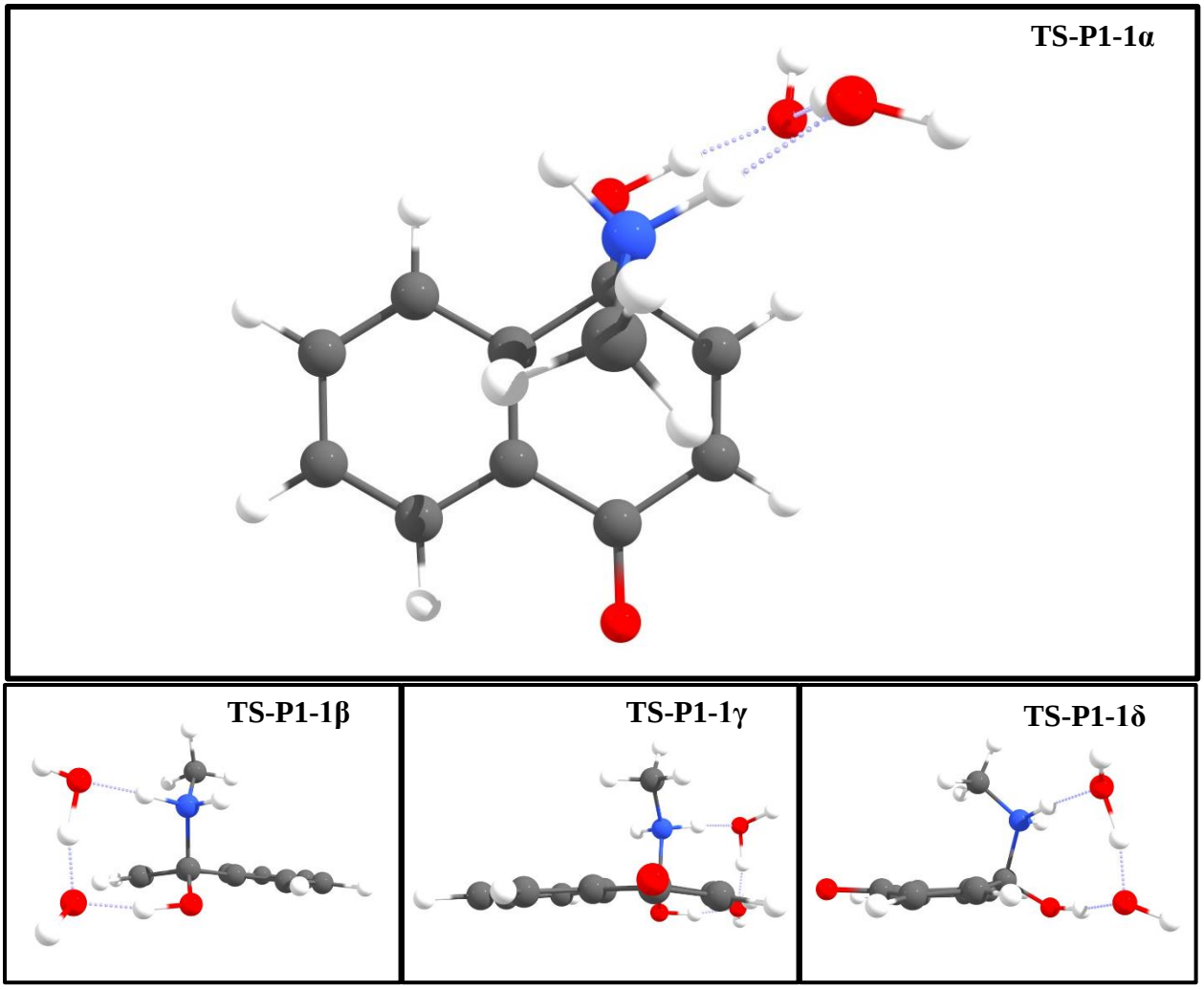


Figure 3.10 Transition state **TS-P1-1**: Lowest energy structure for **R-P1** reaction

As shown in Table 3.2, intermolecular distances C_1–N_a, N_a–H_a, O_w–H_w, O_1–H_x, and C_1–O_1 have fairly consistent values around 1.554 Å, 1.097 Å, 1.121 Å, 1.078 Å, and 1.342 Å, respectively. The remaining intermolecular distances shown in Table 3.2 have enough variation that there does not appear to be a trend.

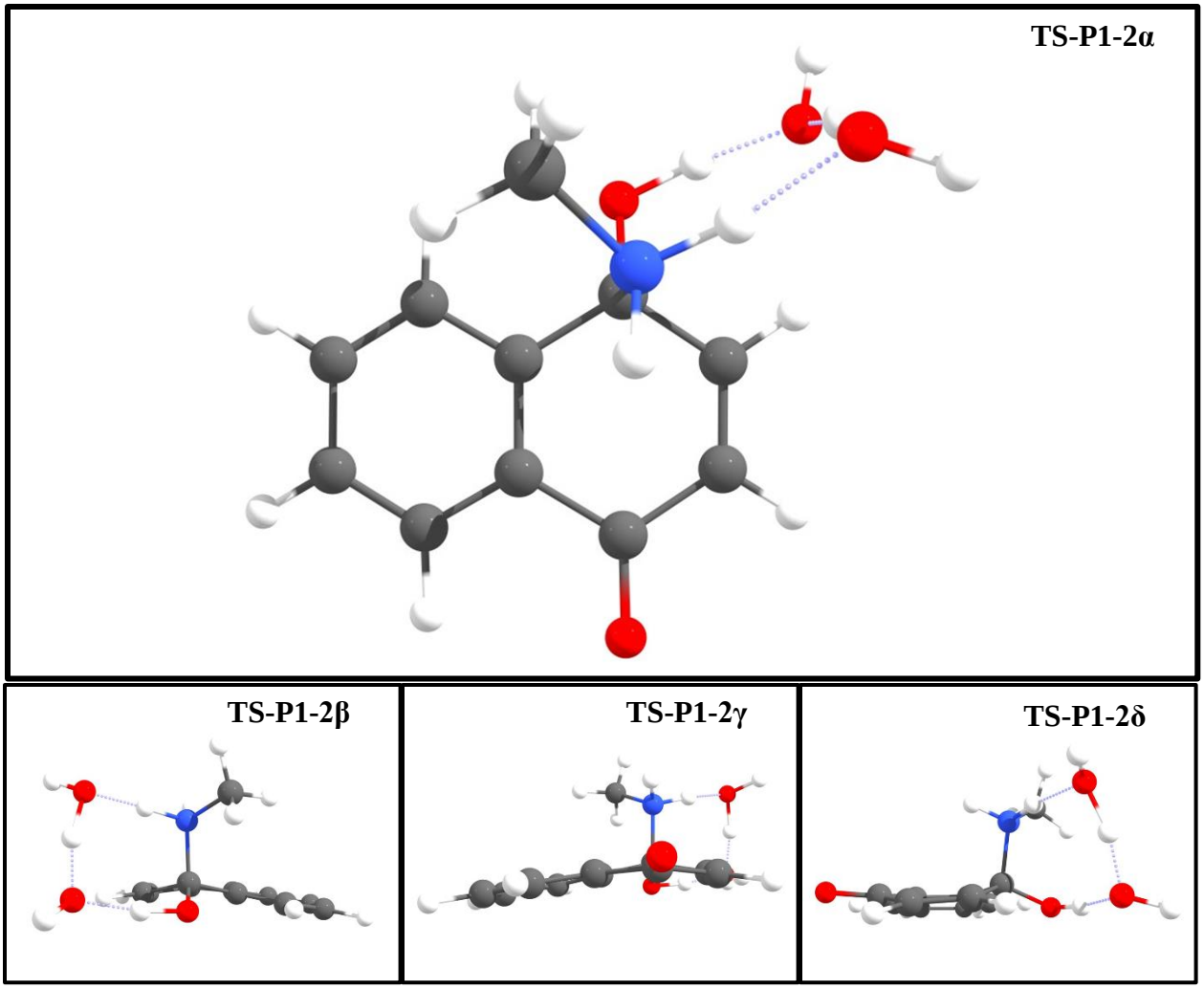


Figure 3.11 Transition state **TS-P1-2**: Second lowest energy structure for **R-P1** reaction

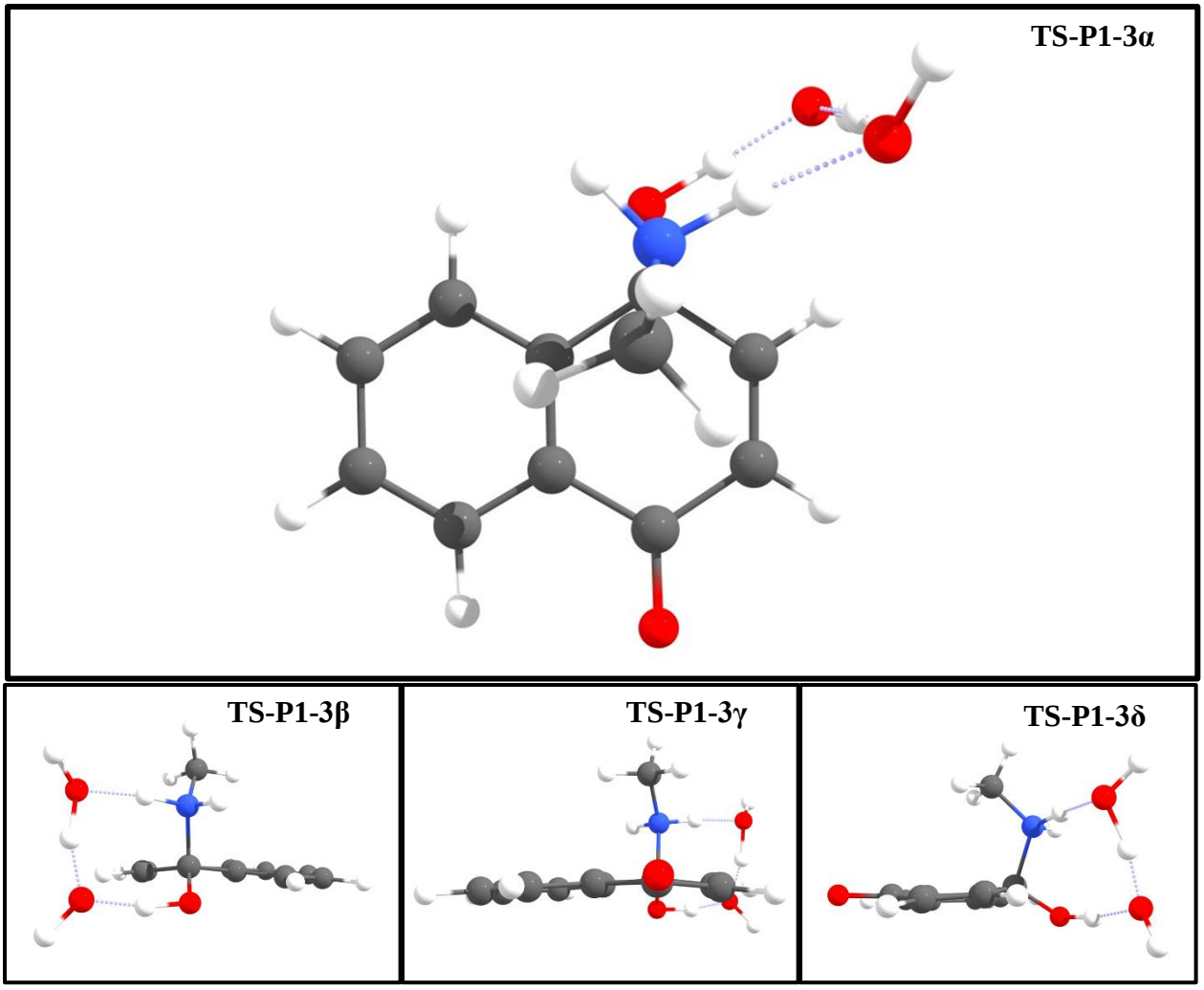


Figure 3.12 Transition state **TS-P1-3**: Third lowest energy structure for **R-P1** reaction

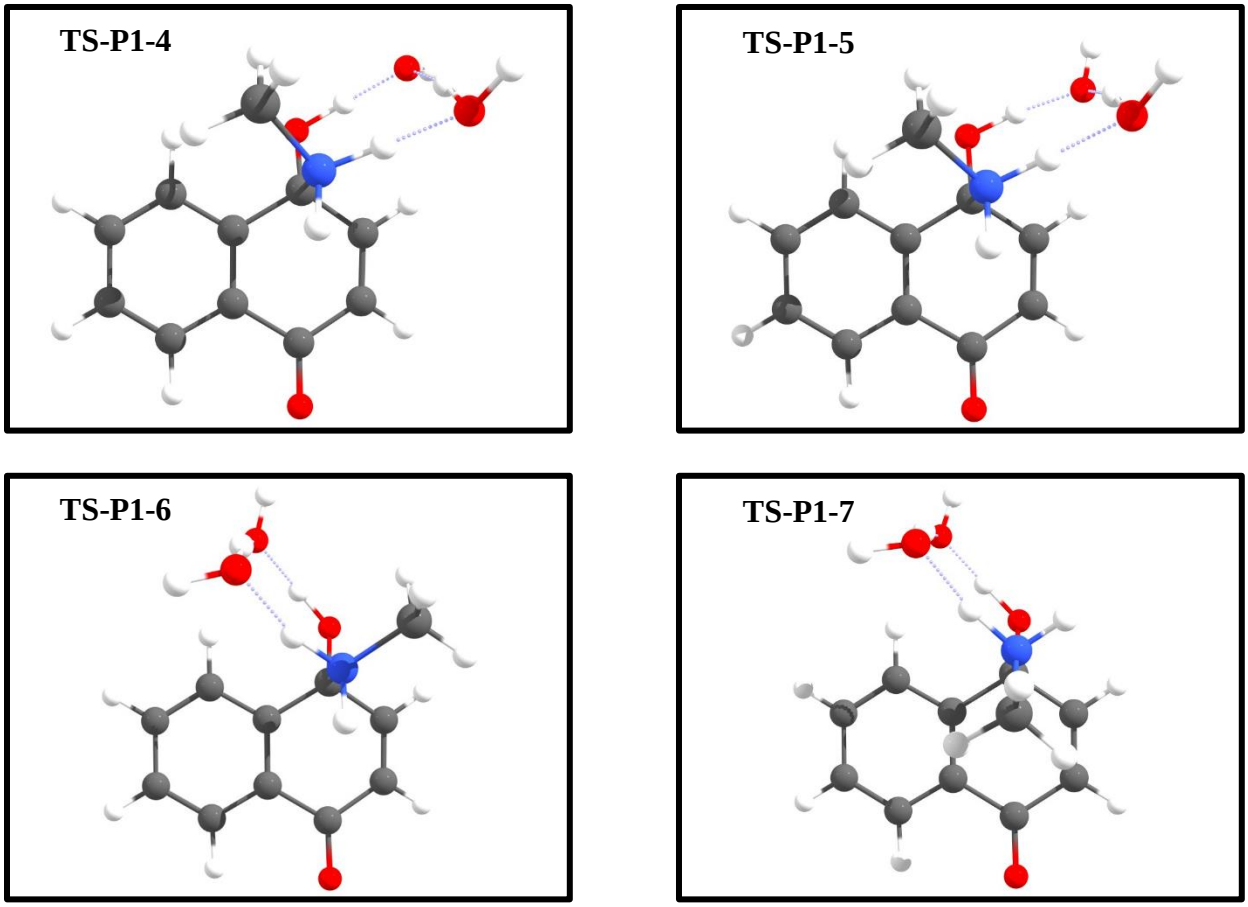


Figure 3.13 Transition states for reaction **R-P1** (energy ranking order 4-7)

3.4.2 1,4-Addition of 1,4-naphthoquinone

Eight different conformers of the transition state were examined, and only five distinct transition states were identified for the **R-P2** reaction. Some important parameters of the optimized transition states are given in Tables 3.3 and 3.4. **TS-P2-1**, **TS-P2-2**, and **TS-P2-3** were the three lowest energy structures optimized for the transition state for the **R-P2** reaction and are shown in Figures 3.14, 3.15, and 3.16. The front views of the remaining optimized transition states are depicted in Figure 3.17.

Table 3.3 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-P2**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-P2-1	7.97	883*i*
TS-P2-2	8.20	1041*i*
TS-P2-3	8.31	990*i*
TS-P2-4	12.95	1077*i*
TS-P2-5	13.61	1233*i*

Table 3.4 Selected internuclear distances (Å) for transition state of reaction **R-P2**

Transition State	C_3—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_1—H_x	C_1—O_1
TS-P2-1	1.490	1.112	1.446	1.115	1.306	1.288	1.125	1.304
TS-P2-2	1.489	1.117	1.430	1.128	1.281	1.262	1.141	1.303
TS-P2-3	1.490	1.107	1.444	1.126	1.291	1.272	1.135	1.303
TS-P2-4	1.510	1.130	1.402	1.132	1.277	1.268	1.137	1.304
TS-P2-5	1.509	1.143	1.374	1.150	1.246	1.231	1.160	1.302

As seen in Table 3.3, the transition state **TS-P2-1** was the lowest gas-phase barrier height of 7.97 kcal/mol when compared to that of the reactants. The next two transition states **TS-P1-2** and **TS-P2-3** had gas-phase barrier heights of 8.20 kcal/mol and 8.31 kcal/mol which only have a less than 1 kcal/mol difference to **TS-P2-1**. The remaining transition states in Table 3.3 are greater than 3 kcal/mol relative to **TS-P2-1**. As seen in Table 3.3, the imaginary frequencies that were observed ranges from 883*i* cm^{-1} to 1233*i* cm^{-1}.

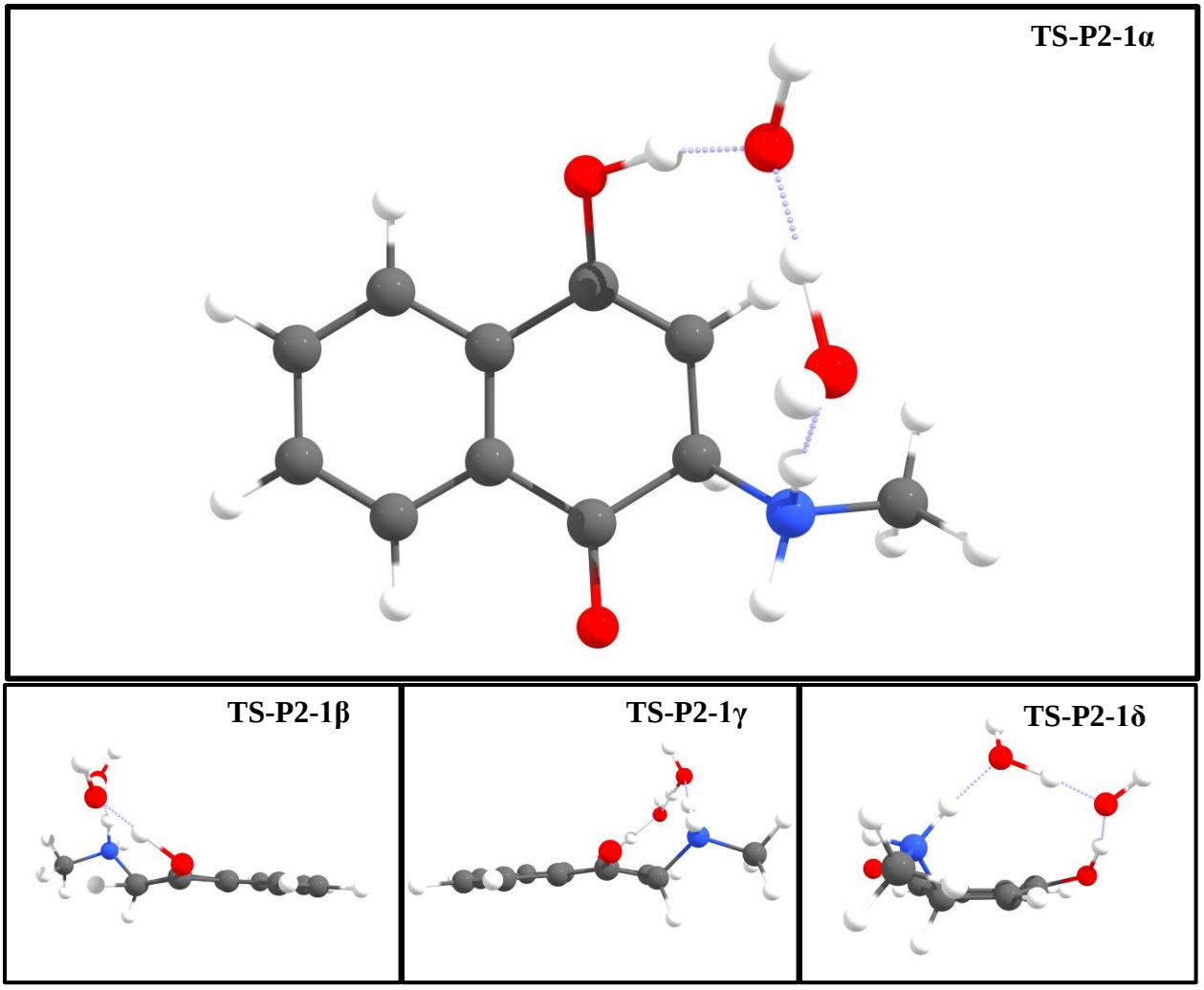


Figure 3.14 Transition state **TS-P2-1**: Lowest energy structure for **R-P2** reaction

As shown in Table 3.4, intermolecular distances C_3–N_a, N_a–H_a, O_w–H_w, O_1–H_x, and C_1–O_1 have fairly consistent values around 1.498 Å, 1.122 Å, 1.130 Å, 1.140 Å, and 1.303 Å, respectively. The remaining intermolecular distances have enough variation to not have a trend.

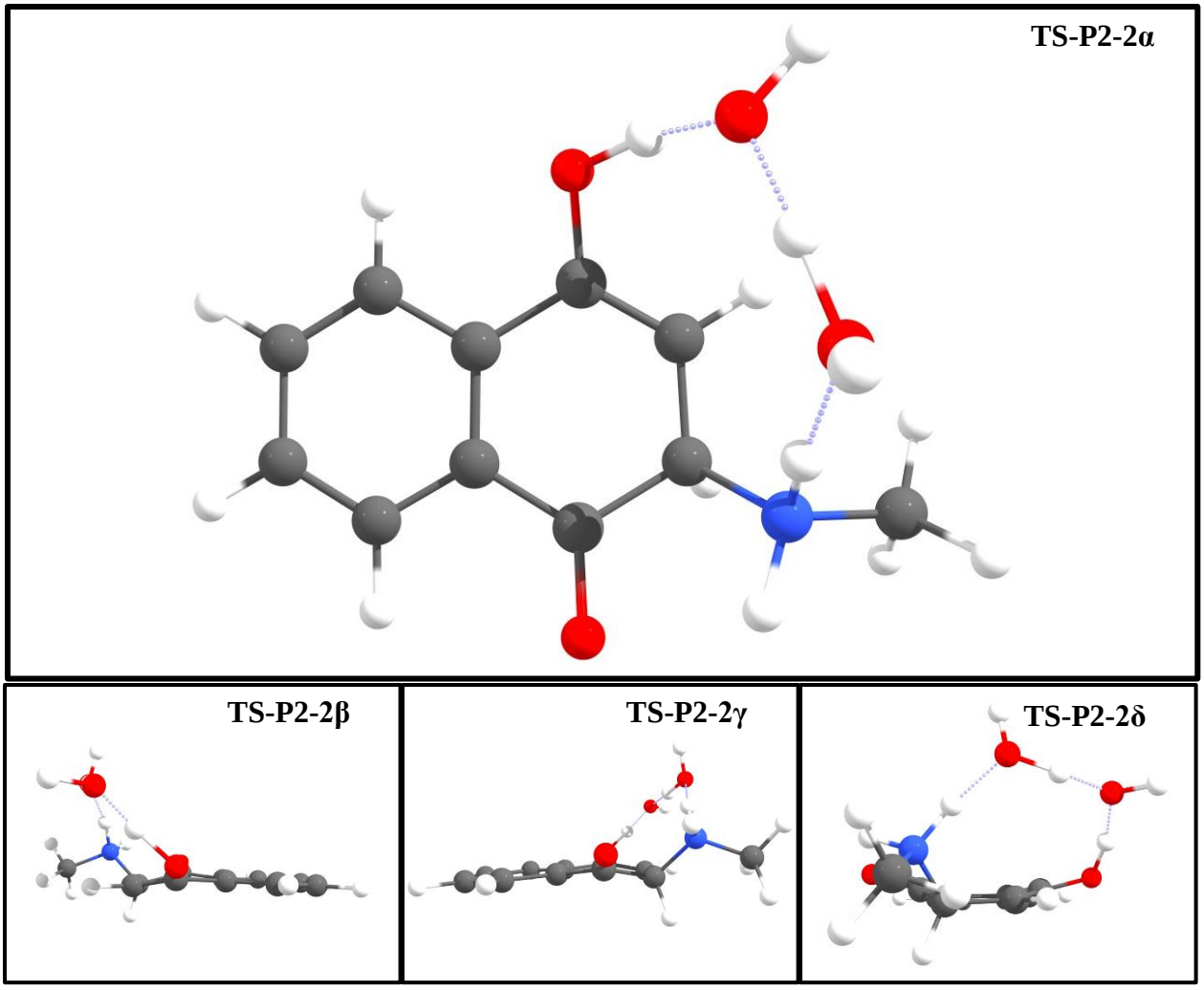


Figure 3.15 Transition state **TS-P2-2**: Second lowest energy structure for **R-P2** reaction

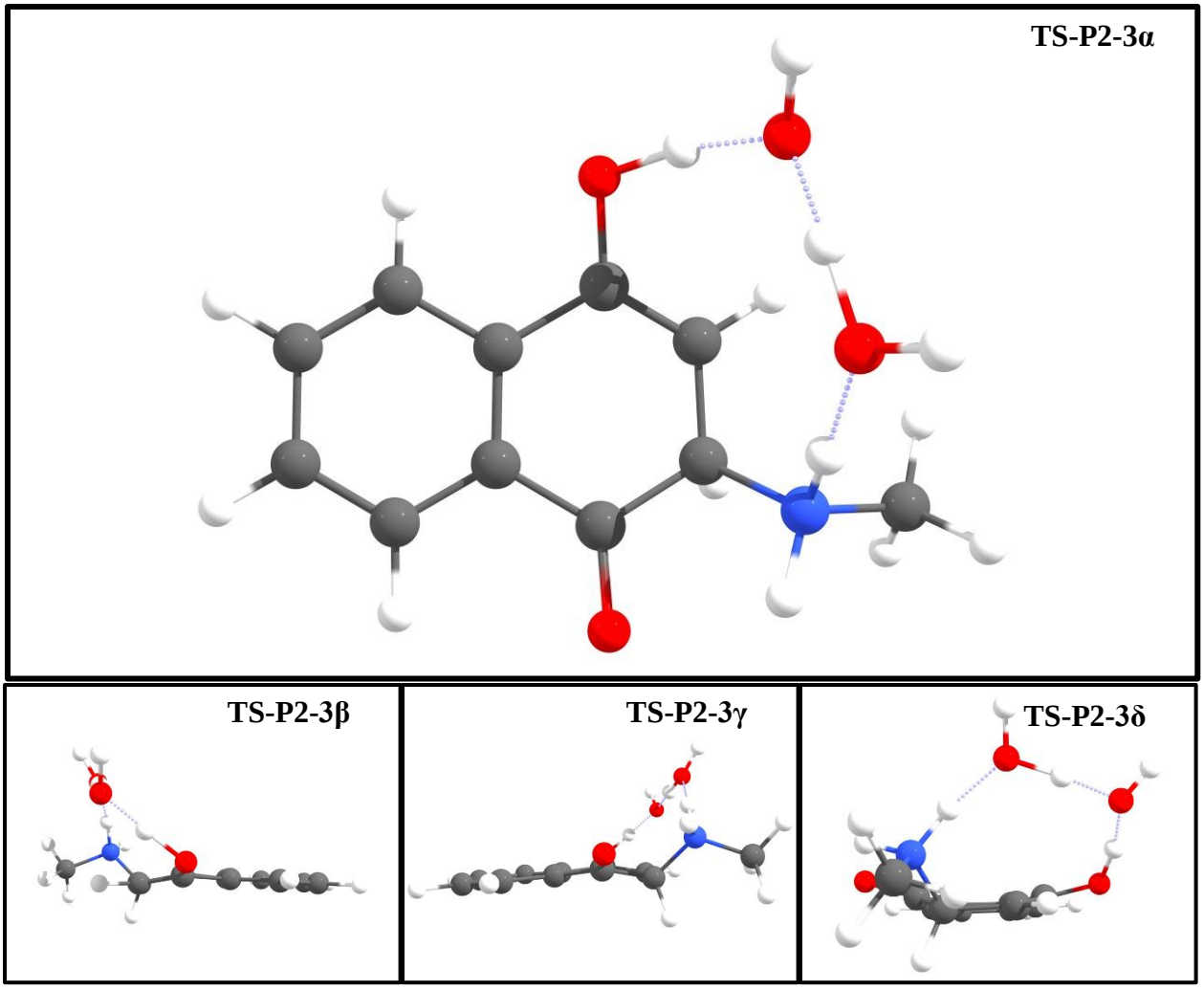


Figure 3.16 Transition state **TS-P2-3**: Third lowest energy structure for **R-P2** reaction

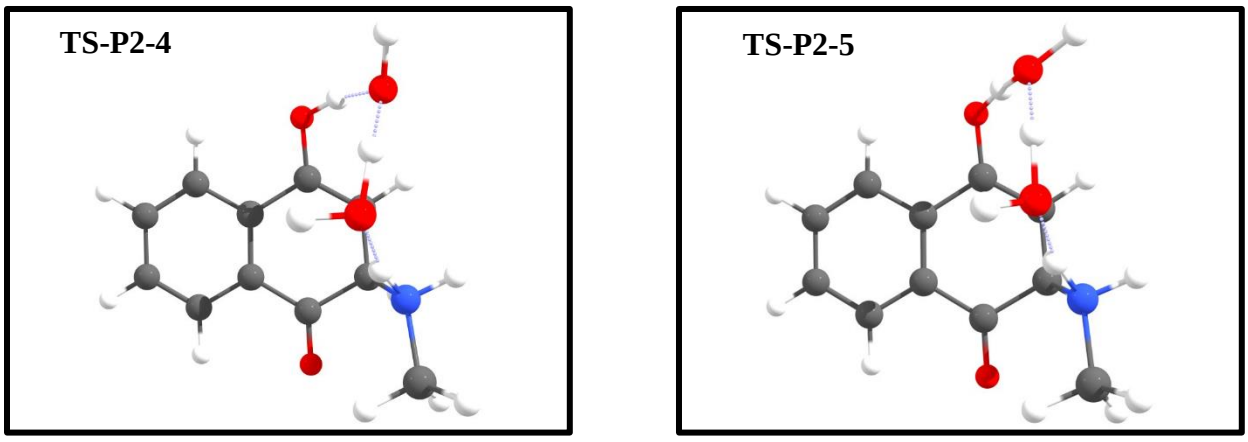


Figure 3.17 Transition states for reaction **R-P2** (energy ranking order 4-5)

3.5 Energy diagram for the reaction between PNQ and methylamine

Once again, each reaction pathway has reactants, reactant complexes, transition states, and products that must be examined to understand the overall reactivity of the naphthoquinone toward the amino group of methylamine. As a result, all the individual stages of the reaction pathway between 1,4-naphthoquinone and methylamine has been investigated. Now, it is necessary to consider the important information from each section that examined the individual stages.

The lowest gas-phase barrier height structure of 1,4-naphthoquinone and the two water molecules with methylamine as a trimer in section 3.2 were utilized to represent the energy of the reactants. In addition, the energy of the reactants was used as a reference (i.e., having a value of 0.00 kcal/mol), and all other structures have energy values relative to it. Next, the transition states were examined for each possible reaction pathway. The lowest gas-phase barrier heights of the transition states for the **R-P1** and **R-P2** reactions are 8.87 kcal/mol and 7.97 kcal/mol, respectively. From these values, the **R-P2** reaction, 1,4-addition, is the most likely pathway for the reaction to occur. However, since both have a less than 1 kcal/mol difference, both reaction pathways could occur and the **R-P2** reaction is only a little more likely. After determining this, one will take the lowest gas-phase barrier height of the products for the **R-P2** reaction and the water dimer calculated in section 3.3 to represent the energy of the products in the overall reaction pathway. The relative energy of the products to the reactants was determined to be 3.79 kcal/mol. Another stage examined in the reaction pathway was the reactant complex. The lowest energy structure for the reactant complexes was determined to be -6.19 kcal/mol relative to the reactants. From this value, the difference between the transition state for the **R-P2** reaction and

the reactant complex can be calculated. The relative energy difference is 14.16 kcal/mol and would give a more accurate representation of the barrier height for the reaction occurring in solution. Using this information, the energy diagram of the reaction was constructed and is shown in Figure 3.18.

The product **P-P2-1**, which is represented in Figure 3.18, is 1.57 kcal/mol lower in energy than product **P-P1-1**. These energy values suggest that the product **P-P2-1** is the lowest energy product and is the most stable product conformation.

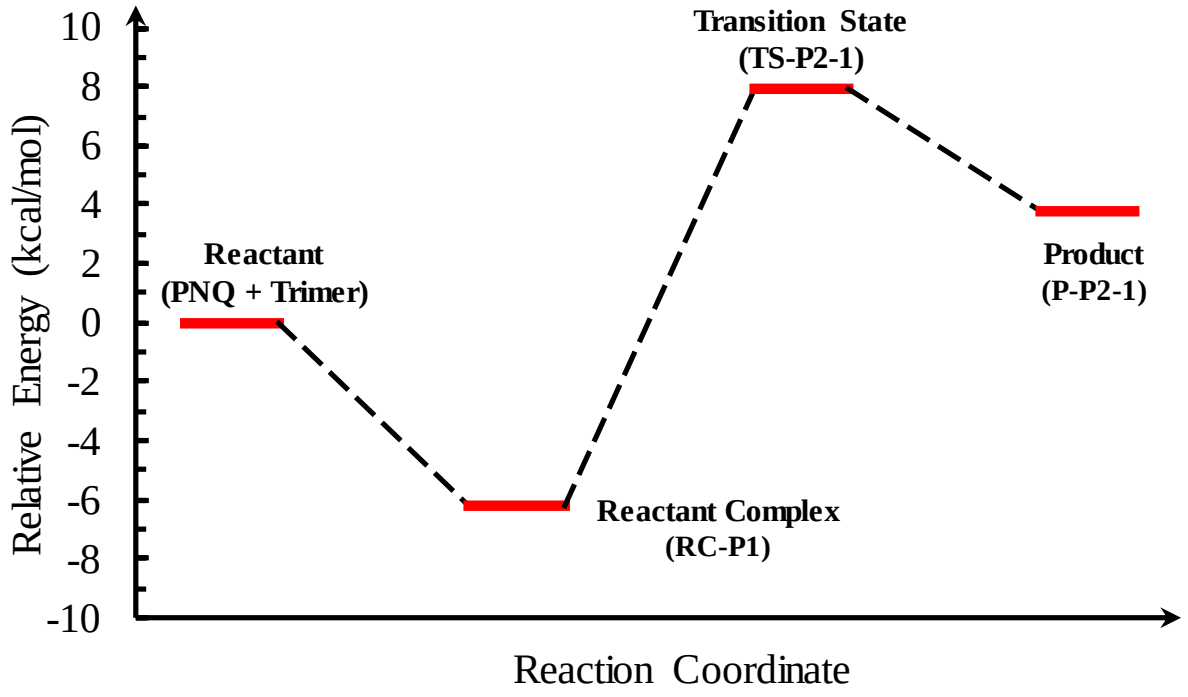


Figure 3.18 Energy diagram for the reaction between 1,4-naphthoquinone and methylamine in the presence of two water molecules

CHAPTER 4

REACTIVITY OF 1,2-NAPHTHOQUINONE

4.1 Introduction

The last reaction investigated was the first step of the reaction between 1,2-naphthoquinone or *ortho*-naphthoquinone (ONQ) and methylamine, CH_3NH_2. Figure 4.1 depicts the numbering of the carbon atoms on ONQ throughout this study. For the reaction between ONQ and CH_3NH_2, there are four different product isomers that can be formed since there are two unique carbonyl positions and two possible reactions for each carbonyl position. The two unique carbonyl positions are at position 1 and position 2 (Figure 4.1). Therefore, the possible reactions are a 1,2-addition at carbonyl 1 (C1), a 1,4-addition at C1, a 1,2-addition at carbonyl 2 (C2), or a 1,4-addition at C2. Figure 4.2 depicts a general schematic for the possible product isomers that can be formed from the reaction of 1,2-naphthoquinone and CH_3NH_2. All the possible reactions studied for the reaction of 1,2-naphthoquinone and CH_3NH_2, namely 1,2-addition at C1, 1,4-addition at C1, 1,2-addition at C2, and 1,4-addition at C2, are shown in Figures 4.3, 4.4, 4.5, and 4.6, respectively. As stated previously, in each reaction pathway, there are reactants, reactant complexes, transition states, and products that must be examined to understand the overall reactivity of the naphthoquinone toward an amino group. Each of the reactions are labeled **R-Ox** where R stands for reaction, O stands for ONQ, and x=1-4 stands for each possible reaction path. Similarly, the four products are labeled **P-Ox** where P stands for product.

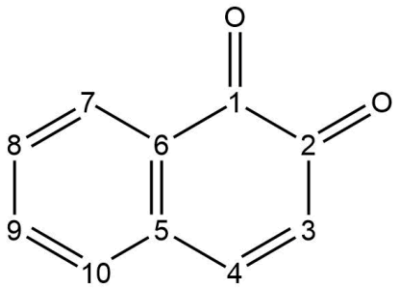


Figure 4.1 Carbon centers numbering of 1,2-naphthoquinone

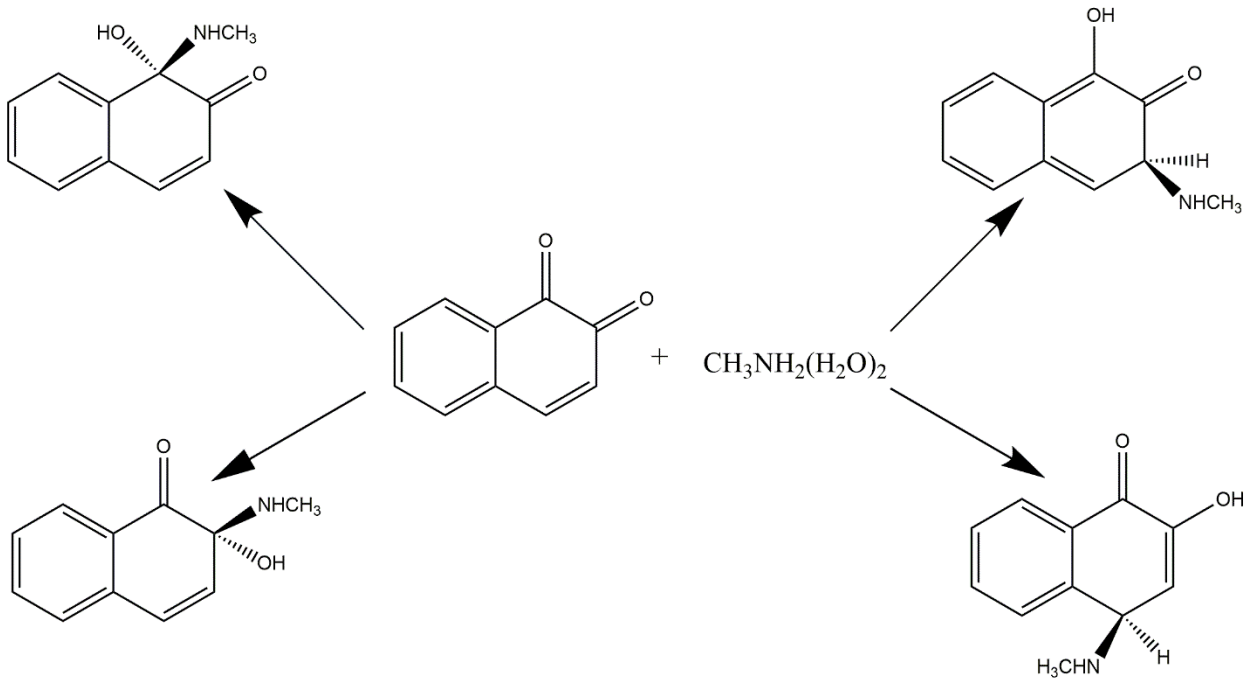
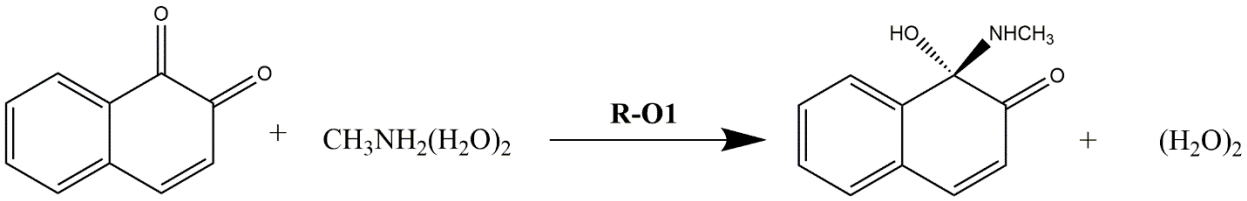
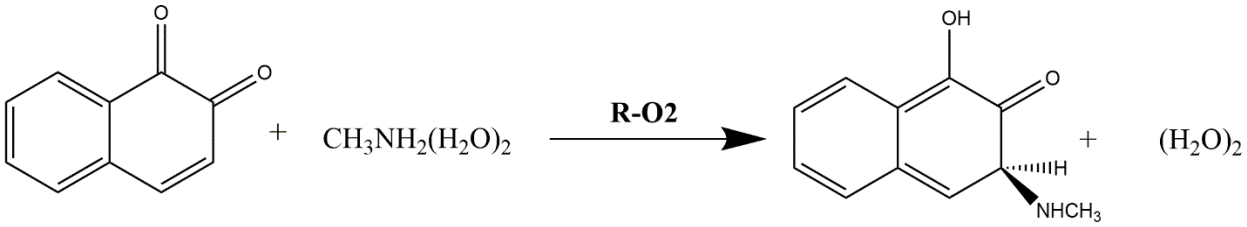


Figure 4.2 Possible reaction pathways for 1,2-naphthoquinone and CH_3NH_2



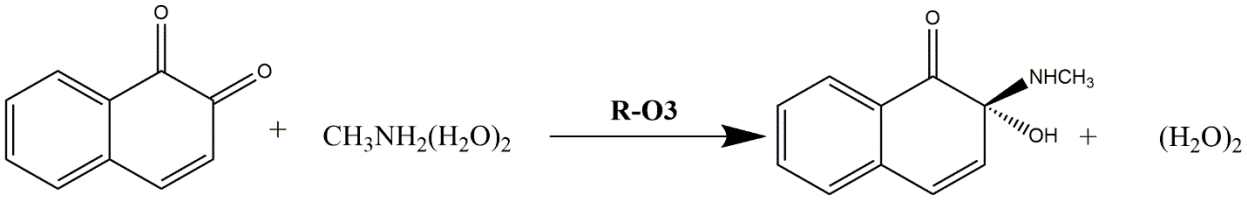
(P-O1)

Figure 4.3 1,2-Addition between 1,2-naphthoquinone and CH_3NH_2 at position 1



(P-O2)

Figure 4.4 1,4-Addition between 1,2-naphthoquinone and CH_3NH_2 at position 1



(P-O3)

Figure 4.5 1,2-Addition between 1,2-naphthoquinone and CH_3NH_2 at position 2

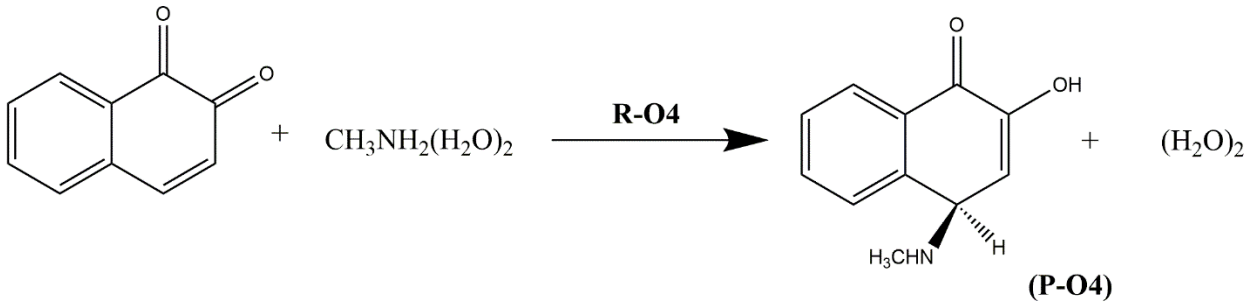


Figure 4.6 1,4-Addition between 1,2-naphthoquinone and CH_3NH_2 at position 2

4.2 Structure and properties of the reactant state (1,2-naphthoquinone)

4.2.1 1,2-Naphthoquinone as a reactant

As stated in the previous chapters, there must be a point of reference to compare the energy of each structure with that of another structure, and this point of reference will be the energy values of the reactants. The first stage of the reactant state will always be the naphthoquinone of interest, and for Chapter 4, this reactant is 1,2-naphthoquinone. 1,2-naphthoquinone only has one structure that was modeled and optimized. The reactant for 1,2-naphthoquinone is labeled **RE-Ox** where RE stands for reactant state, O stands for ONQ, and x is a number to specify a different conformation. Since there is only one structure, x will only be 1. The optimized structure of 1,2-naphthoquinone is shown in Figure 4.7.

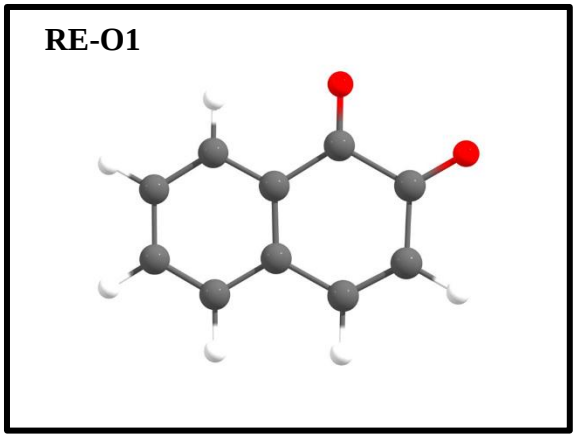


Figure 4.7 **RE-O1**: Optimized structures of 1,2-naphthoquinone

In addition to using the optimized structure of 1,2-naphthoquinone, the energy of the $CH_3HN_2(H_2O)_2$ trimer calculated in section 2.2.2 will be utilized as part of the reactants for Chapter 4. All structures in this chapter will be relative to 1,2-naphthoquinone and the $CH_3HN_2(H_2O)_2$ trimer unless stated otherwise.

4.2.2 Reactant complexes

As stated in Chapter 2, there is the possibility for considering a complex including all the reactants as the reference energy. In this case, the two water molecules, methylamine and an 1,2-naphthoquinone would form a tetramer. These tetramer complexes would be interesting because they would account for the interactions of all the reactants. By having all the interactions, one could more accurately represent the reaction in solution. Overall, 18 different possible arrangements of the 1,2-naphthoquinone tetramer were investigated with only 7 unique optimized conformations found. The lowest energy tetramer was determined and depicted in Figure 4.8. Other interesting tetramers are shown in Figure 4.9 and give a good idea of how the

molecules within the tetramer likes to orient. Each of these calculations took anywhere from three to eleven days of computation on one processor to determine an optimized structure. The reactant complexes for 1,2-naphthoquinone are labeled **RC-Ox** where RC stands for reactant complex, O stands for ONQ, and x is a number to specify a different conformation. Like in the previous chapters, the reactant complexes are labeled from lowest energy to greatest energy, but not all structures are shown here. Only some interesting tetramers are shown in Figure 4.9, so there will be gaps in the labeling of the tetramers. The remaining tetramers' structures can be found in the appendix.

For the tetramer complex, **RC-O1** was determined to be the most stable structure of the tetramer complex. When compared to 1,2-naphthoquinone and the $CH_3HN_2(H_2O)_2$ trimer complex of the reactants, **RC-O1** has a relative energy of -10.18 kcal/mol. The relative energies of **RC-O2**, **RC-O4**, **RC-O6**, and **RC-O7** in Figure 4.9 with respect to **RC-O1** are 0.06 kcal/mol, 0.89 kcal/mol, 2.63 kcal/mol, and 11.07 kcal/mol, respectively.

By comparing the optimized orientations and their respective energies, it seems that the 1,2-naphthoquinone tetramer likes to orient itself similarly to the tetramers in previous chapters. The two water molecules and methylamine still like to interact as a trimer but that is not their ideal orientation. In the lower energy structures, the hydrogens on the water and methylamine like to orient themselves toward the two oxygen atoms on the 1,2-naphthoquinone. This suggests a stronger interaction as a complete tetramer compared to the naphthoquinones in previous chapters where the waters and methylamine liked to form a trimer first.

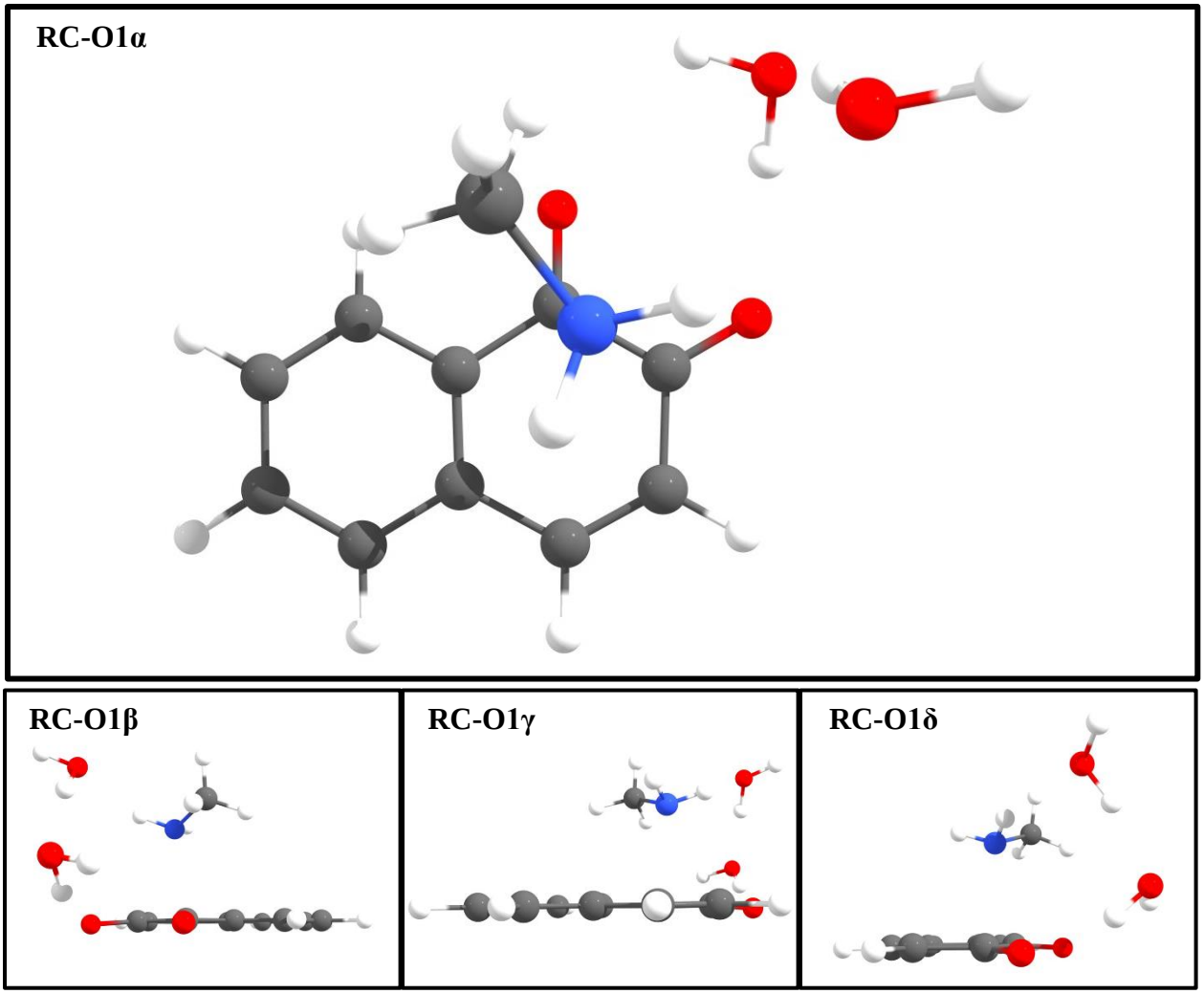


Figure 4.8 Optimized orientation of most stable tetramer complex (1,2-naphthoquinone, methylamine, and two water molecules)

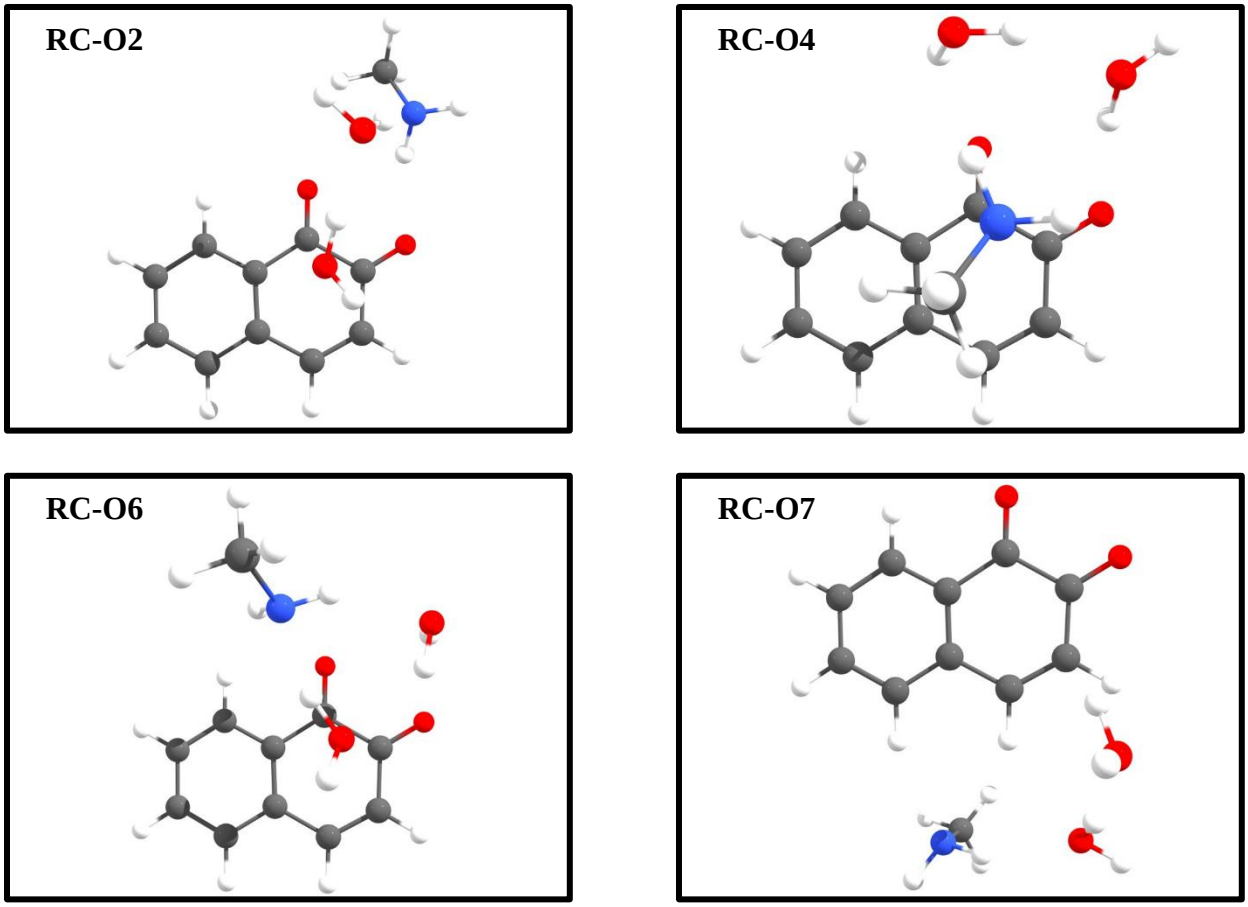


Figure 4.9 Optimized orientations of other tetramer complexes (1,2-naphthoquinone, methylamine, and two water molecules)

4.3 Structure and properties of the product state

4.3.1 1,2-Naphthoquinone and CH_3NH_2 products

The next stage of the reaction between 1,2-naphthoquinone and methylamine depicted in Figure 4.2 is finding the most stable structures of the reaction products. A detailed conformation analysis was carried out for the products in Figure 4.2 where there are 48 possible product conformers based on the four possible reactions. There is a combination of 12 possible orientations for each of the 1,2-additions and 12 possible orientations for each of the 1,4-additions. Each product will have a different IUPAC name, but the factors examined will be the same. The factors examined in these possible conformers are the orientation of the OH functional, formed from the single H atom addition, and the methyl and hydrogen orientations on the binding methylamine. The bound methylamine has a single bond which allows for rotation around the C–N bond, and this rotation was also examined. The calculation time for the optimized geometry of a product conformation is around one to two days. From the 48 possible conformers, 36 distinct product conformations were optimized. Figures 4.10, 4.11, 4.12, and 4.13 represent the four lowest energy products from **R-O1**, **R-O2**, **R-O3**, and **R-O4** reactions, respectively. As stated previously in section 4.1**, P-Ox_1-x_2** where P stands for product, O stands for ONQ, x_1=1-4 stands for each possible reaction path mentioned in section 4.1, and x_2 stands for a distinct conformation.

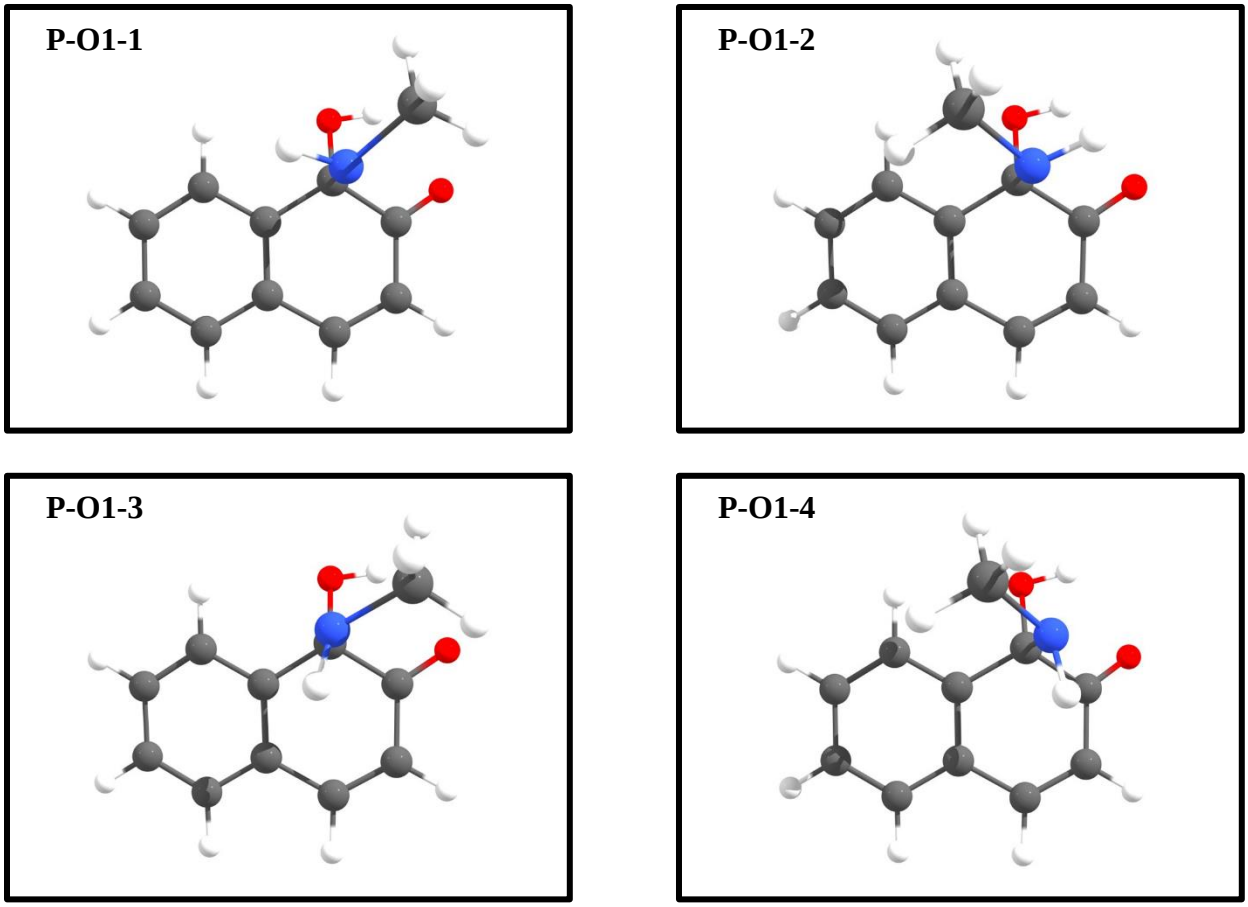


Figure 4.10 **P-O1-1**, **P-O1-2**, **P-O1-3**, and **P-O1-4**: Four lowest energy structures for the product of **R-O1** reaction

Among the four product conformations in Figure 4.10, **P-O1-1** was determined to be the most stable structure for the product of the **R-O1** reaction. The relative energies of **P-O1-2**, **P-O1-3**, and **P-O1-4** with respect to **P-O1-1** are 0.21 kcal/mol, 1.57 kcal/mol, and 2.13 kcal/mol, respectively. For the products of **R-O1**, eight conformations were optimized, and the least stable conformation has a relative energy of 10.62 kcal/mol.

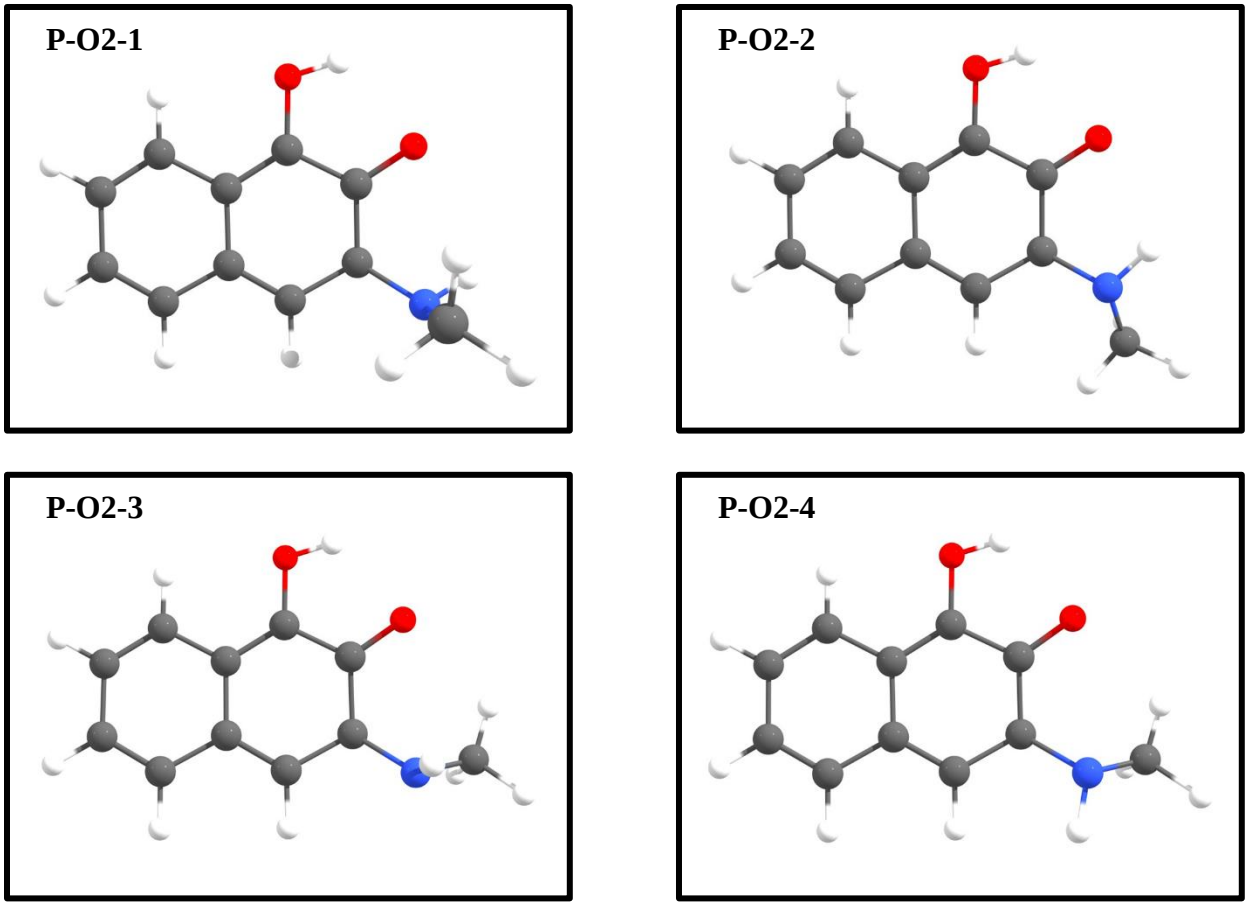


Figure 4.11 **P-O2-1**, **P-O2-2**, **P-O2-3**, and **P-O2-4**: Four lowest energy structures for the product of **R-O2** reaction

Among the four product conformations in Figure 4.11, **P-O2-1** was determined to be the most stable structure for the product of the **R-O2** reaction. The relative energies of **P-O2-2**, **P-O2-3**, and **P-O2-4** with respect to **P-O2-1** are 0.93 kcal/mol, 1.94 kcal/mol, and 3.73 kcal/mol, respectively. For the products of **R-O2**, nine conformations were optimized, and the least stable conformation has a relative energy of 14.32 kcal/mol.

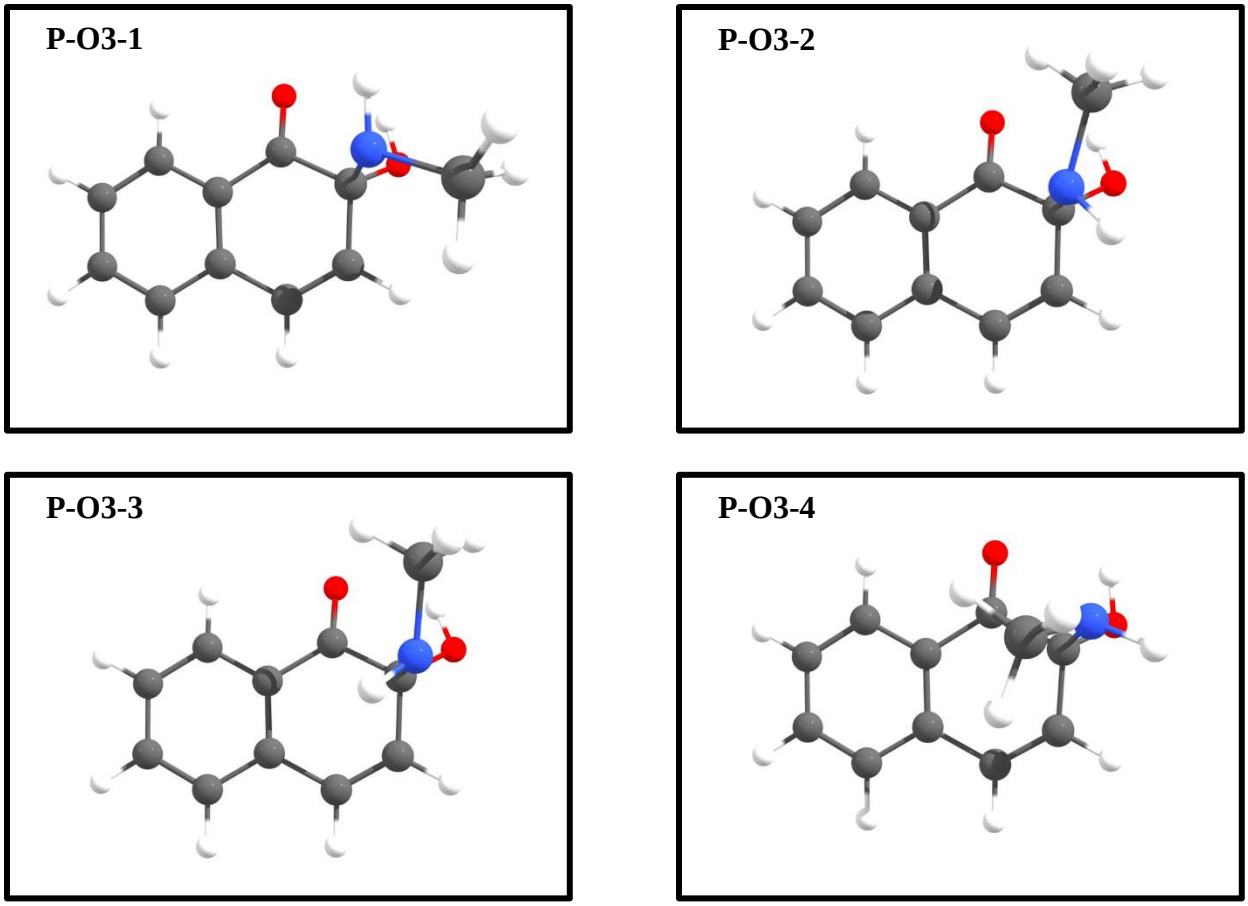


Figure 4.12 **P-O3-1**, **P-O3-2**, **P-O3-3**, and **P-O3-4**: Four lowest energy structures for the product of **R-O3** reaction

Among the four product conformations in Figure 4.12, **P-O3-1** was determined to be the most stable structure for the product of the **R-O3** reaction. The relative energies of P **P-O3-2**, **P-O3-3**, and **P-O3-4** with respect to **P-O3-1** are 0.12 kcal/mol, 1.11 kcal/mol, and 1.39 kcal/mol, respectively. For the products of **R-O3**, ten conformations were optimized, and the least stable conformation has a relative energy of 7.06 kcal/mol.

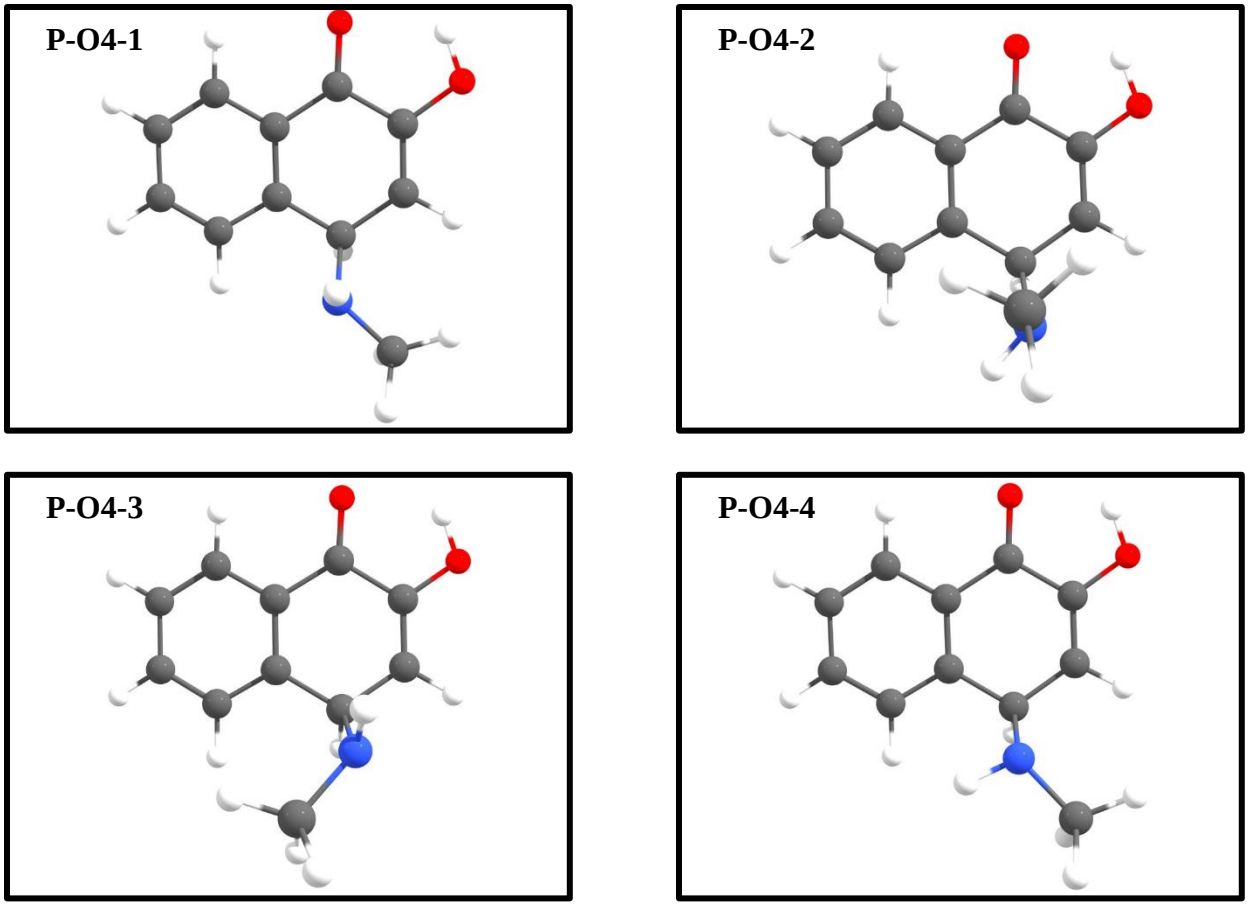


Figure 4.13 **P-O4-1**, **P-O4-2**, **P-O4-3**, and **P-O4-4**: Four lowest energy structures for the product of **R-O4** reaction

Among the four product conformations in Figure 4.13, **P-O4-1** was determined to be the most stable structure for the product of the **R-O4** reaction. The relative energies of **P-O4-2**, **P-O4-3**, and **P-O4-4** with respect to **P-O4-1** are 0.57 kcal/mol, 1.90 kcal/mol, and 3.00 kcal/mol, respectively. For the products of **R-O4**, nine conformations were optimized, and the least stable conformation has a relative energy of 10.96 kcal/mol.

4.4 Analysis of transition states

Once again, the transition state is the most important stage of the reaction pathway because it determines the energy barrier that must be overcome for the reaction to occur. Therefore, it is necessary to determine the most likely transition state for each possible reaction pathways so that one can determine which reaction is most likely to occur. In this study, there is a focus on the first step of the hydrogen transfer from the nucleophile, methylamine, to the carbonyl group at carbon 1 and 2 of 1,2-naphthoquinone as the transition state. To study this transition state, the model described in section 2.4 will be utilized to facilitate the hydrogen transfer.

An analysis was carried out for the transition states of 1,2-addition at C1, 1,2-addition at C2, 1,4-addition at C1, and 1,4-addition at C2. The important factors examined in each transition state in this section are the methyl position on the amine, the location of the hydrogen transfer through the two water molecules, and the position of the hydrogens on the two water molecules. There was a total of 43 transition states examined, and only 32 distinct transition states were optimized. Overall, the calculation times for the optimized geometry of a transition state ranges from two to four days. As for the naming of the structures presented in this study, **TS-Ox_1-x_2** where TS stands for transition state, O stands for ONQ, x_1=1-4 stands for each possible reaction path mentioned in section 4.1, and x_2 stands for a different conformation in that possible reaction path. The energy of the dimer of the two water molecules calculated in section 2.3.2 will be utilized with the products calculated in this section to determine the overall energy of the products.

4.4.1 1,2-Addition at carbonyl 1 of 1,2-naphthoquinone

Sixteen different conformers of the transition state were examined, and only fourteen distinct transition states were identified for the **R-O1** reaction. A summary of some important parameters of the transition states are given in Tables 4.1 and 4.2. As stated previously, the symbols $V^{\ddagger}$ and $\omega^{\ddagger}$ are gas-phase barrier height in kcal/mol and imaginary frequency in cm^{-1}, respectively. The gas-phase barrier height in the tables of this section are relative to the calculated energy of the individual naphthoquinone and $CH_3HN_2(H_2O)_2$ trimer. For Table 4.2, the intermolecular distances presented in the table are in angstroms (Å). The labeling of the atoms in the transition state follows the same structure as depicted in section 2.4.

Table 4.1 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-O1**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-O1-1	1.08	883*i*
TS-O1-2	1.41	813*i*
TS-O1-3	2.00	818*i*
TS-O1-4	5.26	1336*i*
TS-O1-5	5.34	1380*i*
TS-O1-6	5.53	594*i*
TS-O1-7	5.73	1413*i*
TS-O1-8	6.07	1358*i*
TS-O1-9	6.76	1390*i*
TS-O1-10	7.03	611*i*
TS-O1-11	7.04	1354*i*
TS-O1-12	7.15	540*i*
TS-O1-13	7.44	1292*i*
TS-O1-14	9.70	1104*i*

Table 4.2 Selected internuclear distances (Å) for transition state of reaction **R-O1**

Transition State	C_1—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_1—H_x	C_1—O_1
TS-O1-1	1.505	1.089	1.500	1.147	1.246	1.301	1.107	1.352
TS-O1-2	1.507	1.086	1.504	1.141	1.258	1.323	1.097	1.353
TS-O1-3	1.507	1.084	1.495	1.142	1.253	1.328	1.097	1.351
TS-O1-4	1.561	1.150	1.354	1.205	1.185	1.176	1.220	1.317
TS-O1-5	1.559	1.164	1.336	1.200	1.195	1.172	1.223	1.316
TS-O1-6	1.554	1.100	1.463	1.113	1.292	1.358	1.077	1.326
TS-O1-7	1.497	1.245	1.246	1.120	1.283	1.179	1.212	1.348
TS-O1-8	1.499	1.293	1.198	1.119	1.288	1.135	1.263	1.343
TS-O1-9	1.546	1.188	1.303	1.194	1.195	1.145	1.256	1.323
TS-O1-10	1.559	1.096	1.468	1.117	1.288	1.365	1.073	1.326
TS-O1-11	1.558	1.163	1.345	1.167	1.223	1.215	1.179	1.320
TS-O1-12	1.546	1.100	1.471	1.123	1.277	1.429	1.042	1.334
TS-O1-13	1.563	1.127	1.390	1.182	1.210	1.226	1.173	1.319
TS-O1-14	1.502	1.151	1.373	1.138	1.264	1.283	1.121	1.354

TS-O1-1, **TS-O1-2**, and **TS-O1-3** were the three lowest energy structures optimized for the transition state of the **R-O1** reaction and are shown in Figures 4.14, 4.15, and 4.16. The front views of the remaining optimized transition states are depicted in Figures 4.17 and 4.18.

As seen in Table 4.1, the transition state **TS-O1-1** was the lowest gas-phase barrier height of 1.08 kcal/mol when compared to that of the reactants. The next two transition states **TS-O1-2** and **TS-O1-3** had gas-phase barrier heights of 1.41 kcal/mol and 2.00 kcal/mol which only have a less than 1 kcal/mol difference to the **TS-O1-1**. The remaining transition states in Table 4.1 are all greater in energy by 4 kcal/mol with **TS-O1-14** having the highest gas-phase barrier at 9.70 kcal/mol.

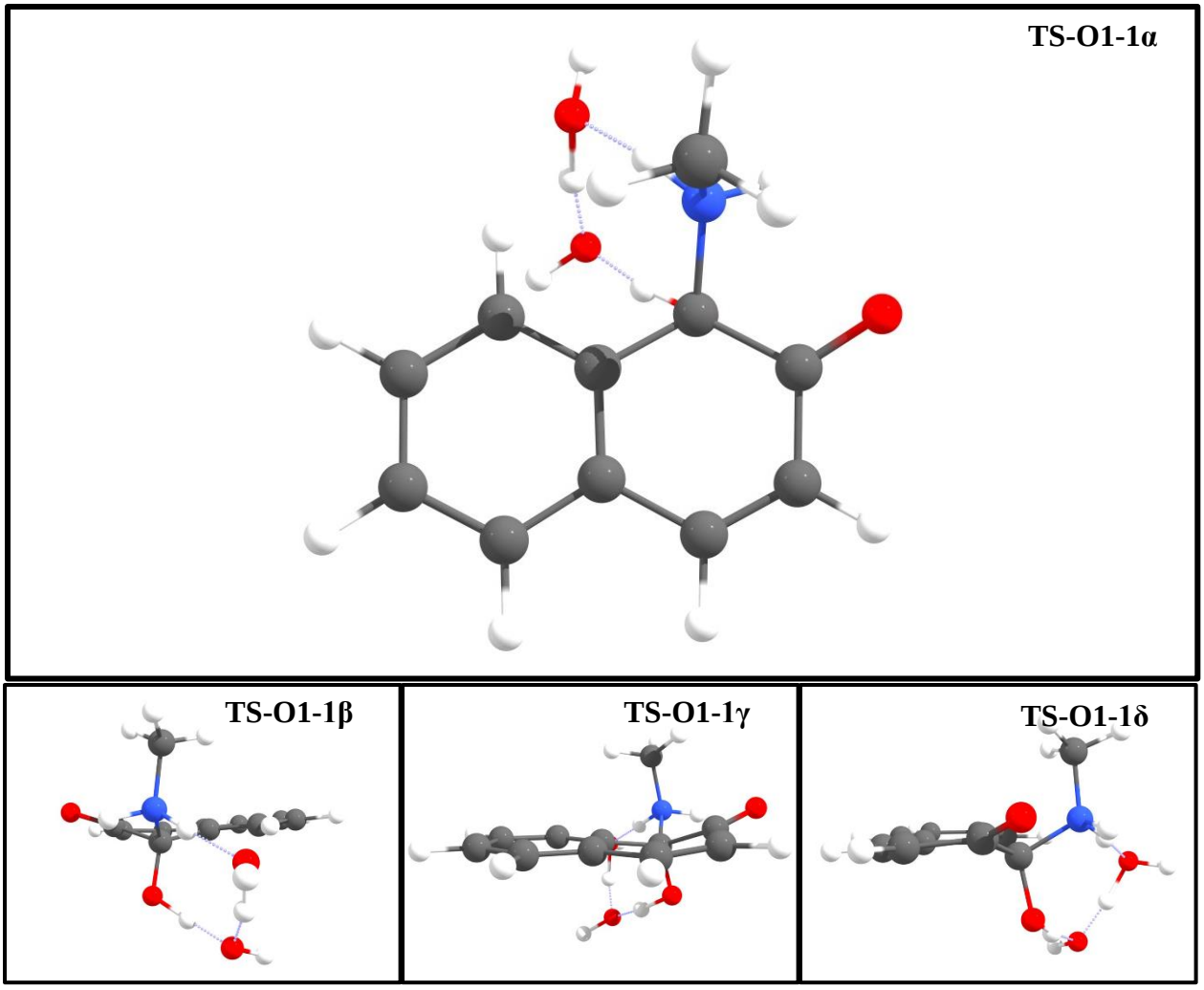


Figure 4.14 Transition state **TS-O1-1**: Lowest energy structure for **R-O1** reaction

As seen in Table 4.1, there are three sets of imaginary frequencies that were observed. The first set includes transition states **TS-O1-1** to **3** with imaginary frequencies around 800*i* cm^{-1}. The second set includes transition states **TS-O1-4 to 5**, **TS-O1-7 to 9**, **TS-O1-11**, and **TS-O1-13 to 14** with imaginary frequencies ranging from 1104*i* cm^{-1} to 1390*i* cm^{-1}. The third set includes **TS-O1-6**, **TS-O1-10**, and **TS-O1-12** with imaginary frequencies around 600*i* cm^{-1}.

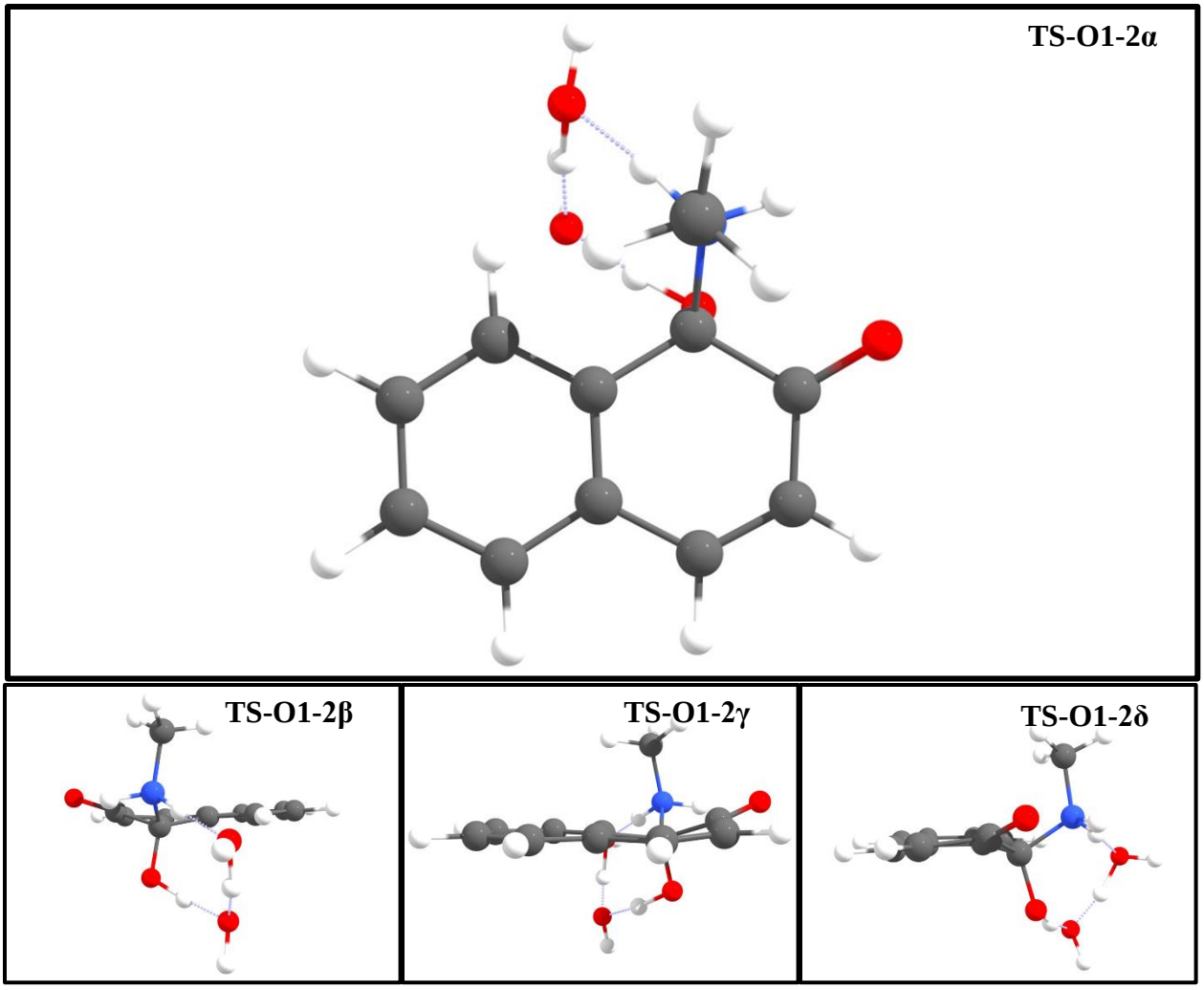


Figure 4.15 Transition state **TS-O1-2**: Second lowest energy structure for **R-O1** reaction

As shown in Table 4.2, there are few intermolecular distances that have consistency that can be seen. Some consistency can be seen when the intermolecular distances are divided into two different sets. The first set includes transition states **TS-O1-1** to **3**, **TS-O1-7** to **8**, and **TS-O1-14**. The second set includes the remaining transition states. In the first set, the C_1–N_a and C_1–O_1 have fairly consistent values around 1.503 Å and 1.350 Å, respectively. In the second set, the C_1–N_a and C_1–O_1 have fairly consistent values around 1.556 Å and 1.323 Å, respectively. The

remaining intermolecular distances shown in Table 4.2 have enough variation that there does not appear to be a trend.

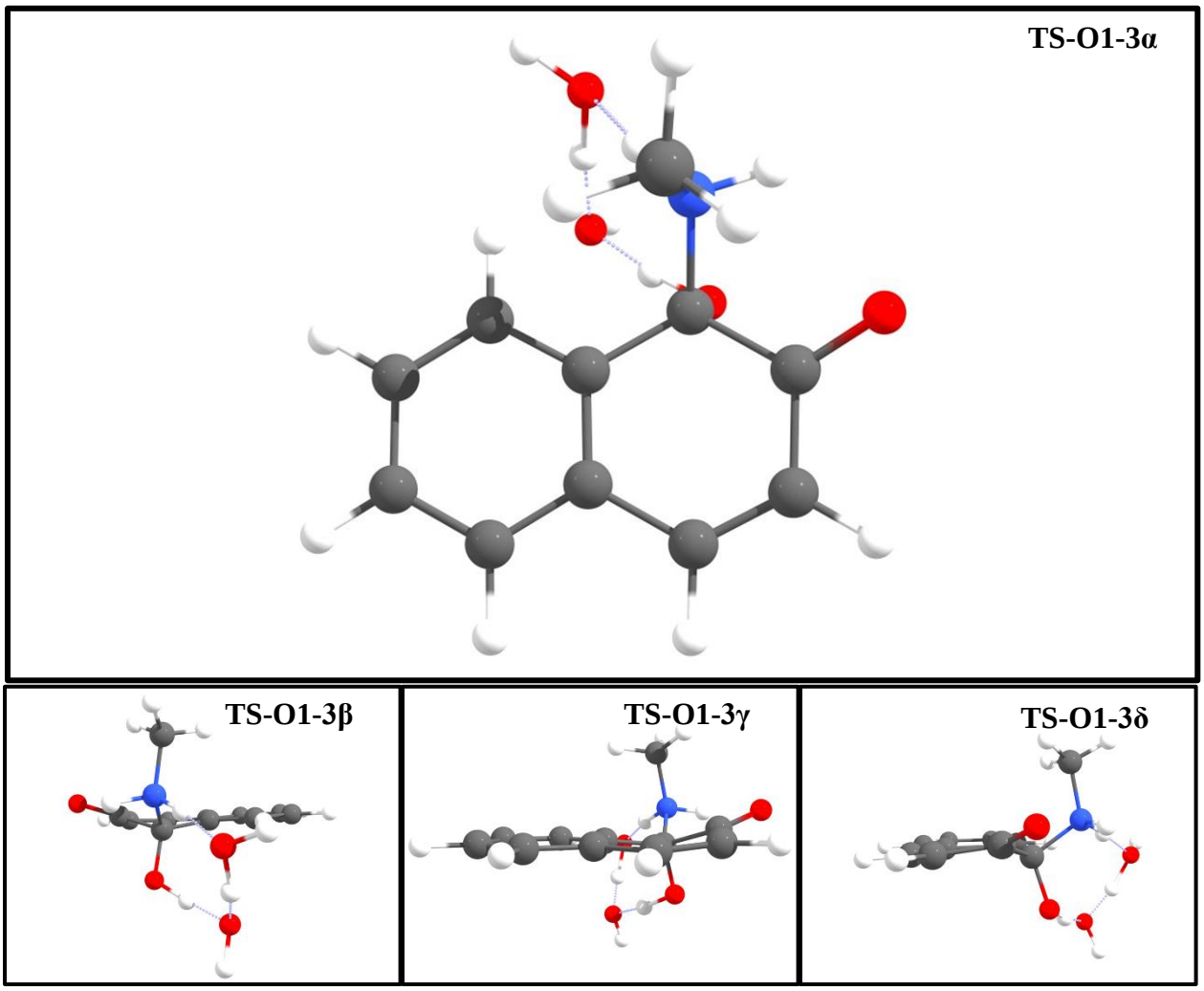


Figure 4.16 Transition state **TS-O1-3**: Third lowest energy structure for **R-O1** reaction

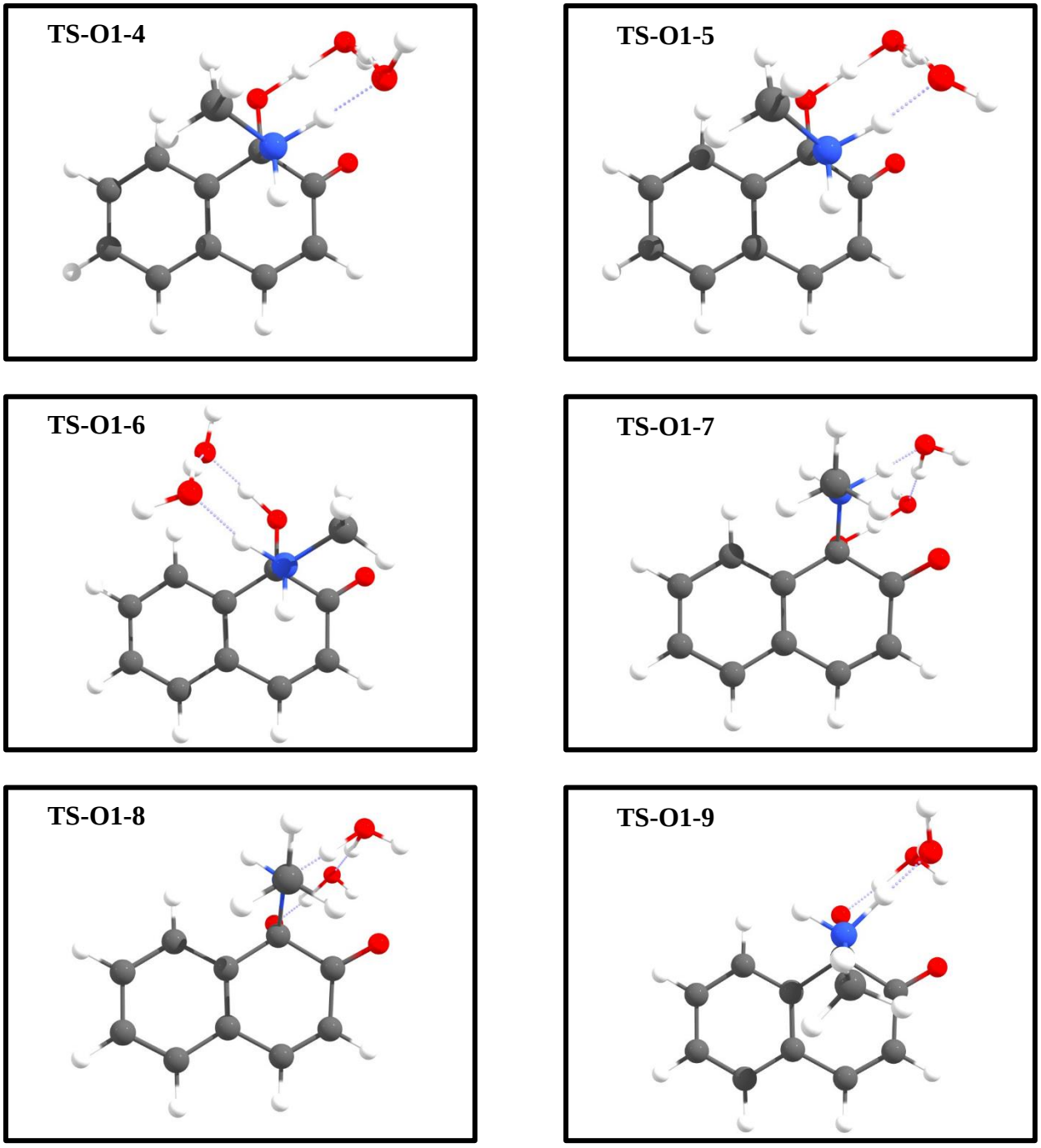


Figure 4.17 Transition states for reaction **R-O1** (energy ranking order 4-9)

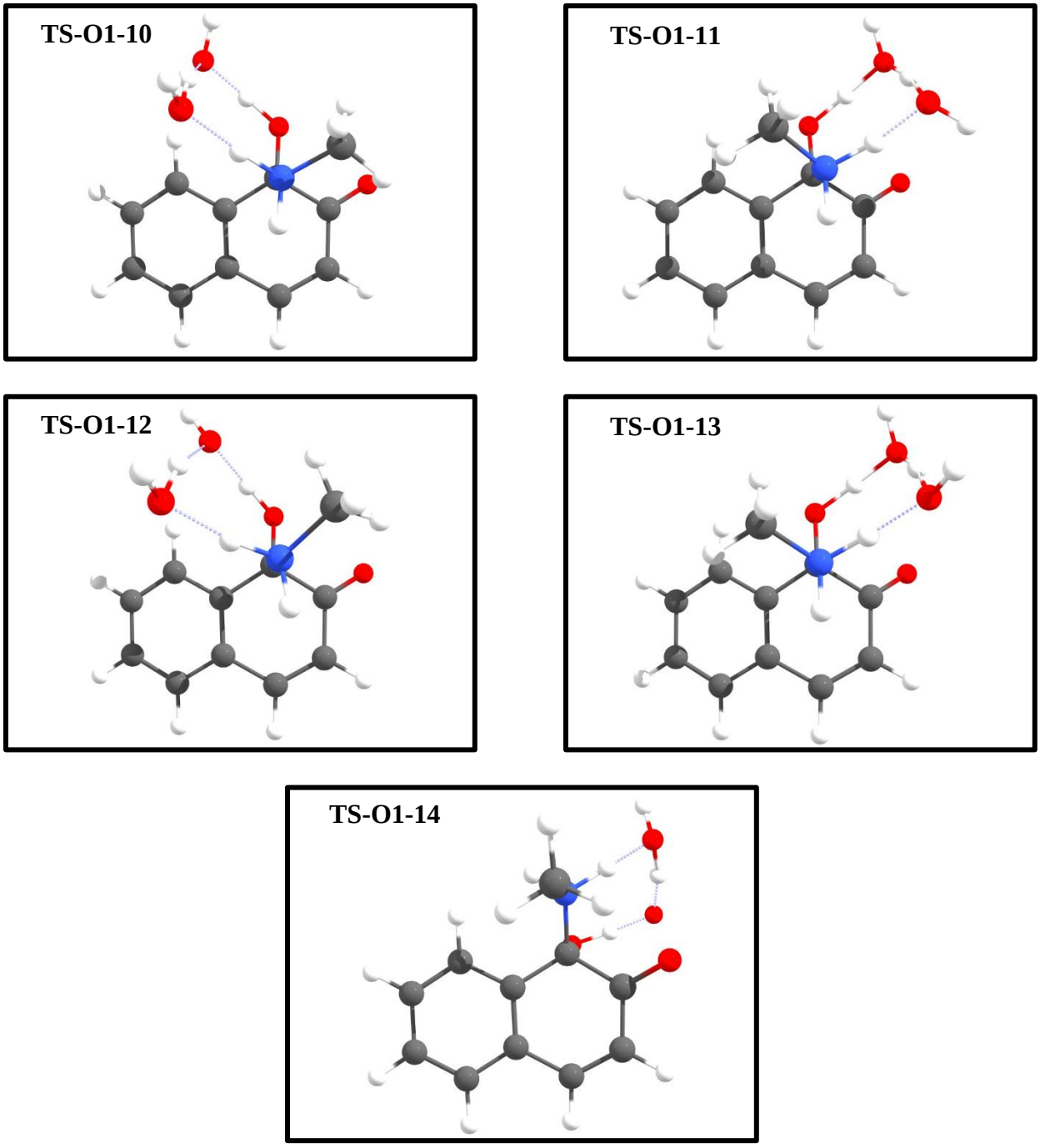


Figure 4.18 Transition states for reaction **R-O1** (energy ranking order 10-14)

4.4.2 1,4-Addition at carbonyl 1 of 1,2-naphthoquinone

Nine different conformers of the transition state were examined, and only six distinct transition states were identified for the **R-O2** reaction. A summary of some important parameters of the transition states are given in Tables 4.3 and 4.4.

Table 4.3 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-O2**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-O2-1	25.01	1190*i*
TS-O2-2	25.14	1313*i*
TS-O2-3	25.68	1015*i*
TS-O2-4	27.51	1292*i*
TS-O2-5	28.47	1211*i*
TS-O2-6	29.20	1405*i*

Table 4.4 Selected internuclear distances (Å) for transition state of reaction **R-O2**

Transition State	C_3—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_1—H_x	C_1—O_1
TS-O2-1	1.487	1.342	1.152	1.170	1.232	1.047	1.433	1.267
TS-O2-2	1.502	1.287	1.195	1.179	1.215	1.059	1.396	1.267
TS-O2-3	1.482	1.410	1.108	1.173	1.225	1.052	1.431	1.268
TS-O2-4	1.499	1.321	1.167	1.180	1.213	1.076	1.369	1.270
TS-O2-5	1.496	1.332	1.166	1.155	1.241	1.059	1.404	1.268
TS-O2-6*	1.406	1.263	1.209	1.161	1.231	1.120	1.281	1.311

***** Does not follow same labeling as other structures (C_3 will be O_2 in this structure)

TS-O2-1, **TS-O2-2**, and **TS-O2-3** were the three lowest energy structures optimized for the transition state of the **R-O2** reaction and are shown in Figures 4.19, 4.20, and 4.21. The front views of the remaining optimized transition states are depicted in Figure 4.22.

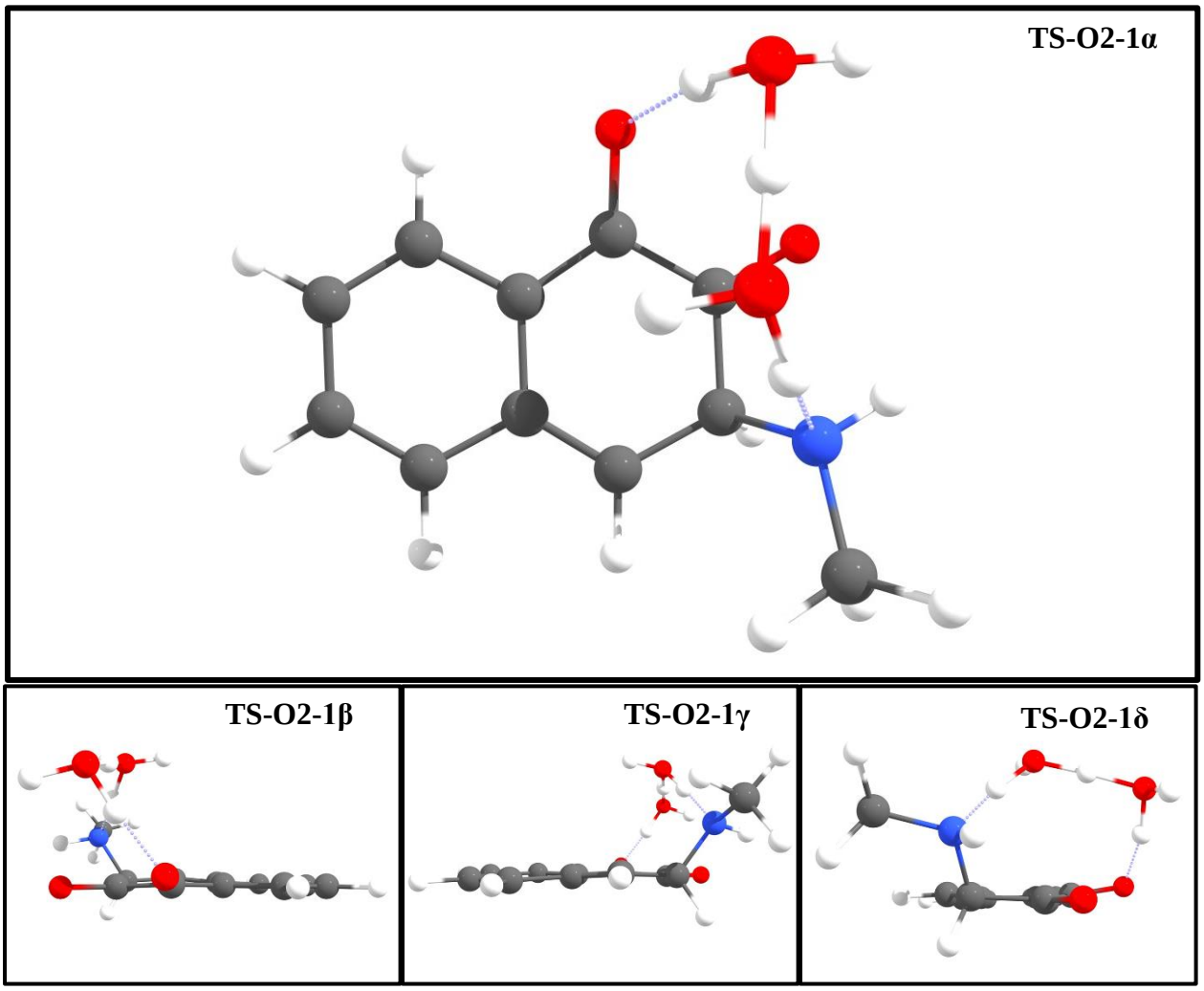


Figure 4.19 Transition state **TS-O2-1**: Lowest energy structure for **R-O2** reaction

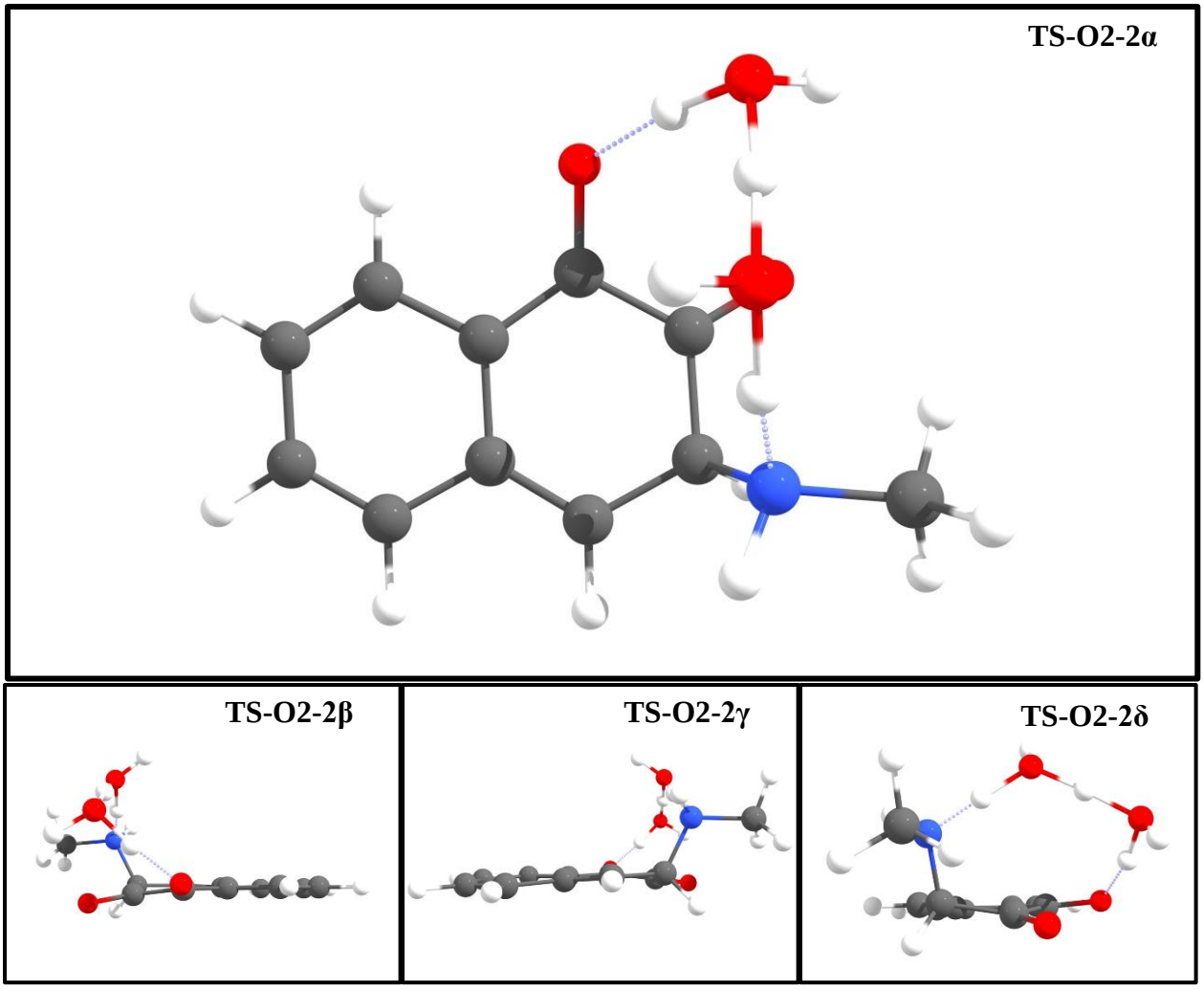


Figure 4.20 Transition state **TS-O2-2**: Second lowest energy structure for **R-O2** reaction

As seen in Table 4.3, the transition state **TS-O2-1** was the lowest gas-phase barrier height of 25.01 kcal/mol when compared to that of the reactants. The next two transition states **TS-O2-2** and **TS-O2-3** had gas-phase barrier heights of 25.14 kcal/mol and 25.68 kcal/mol which only have a less than 1 kcal/mol difference to the **TS-O2-1**. The remaining transition states in Table 4.3 are all greater in energy by 2.50 kcal/mol with **TS-O2-6** having the highest gas-phase barrier at 29.20 kcal/mol. As seen in Table 4.4, the imaginary frequencies of the transition states range from 1015*i* cm^{-1} to 1405*i* cm^{-1}.

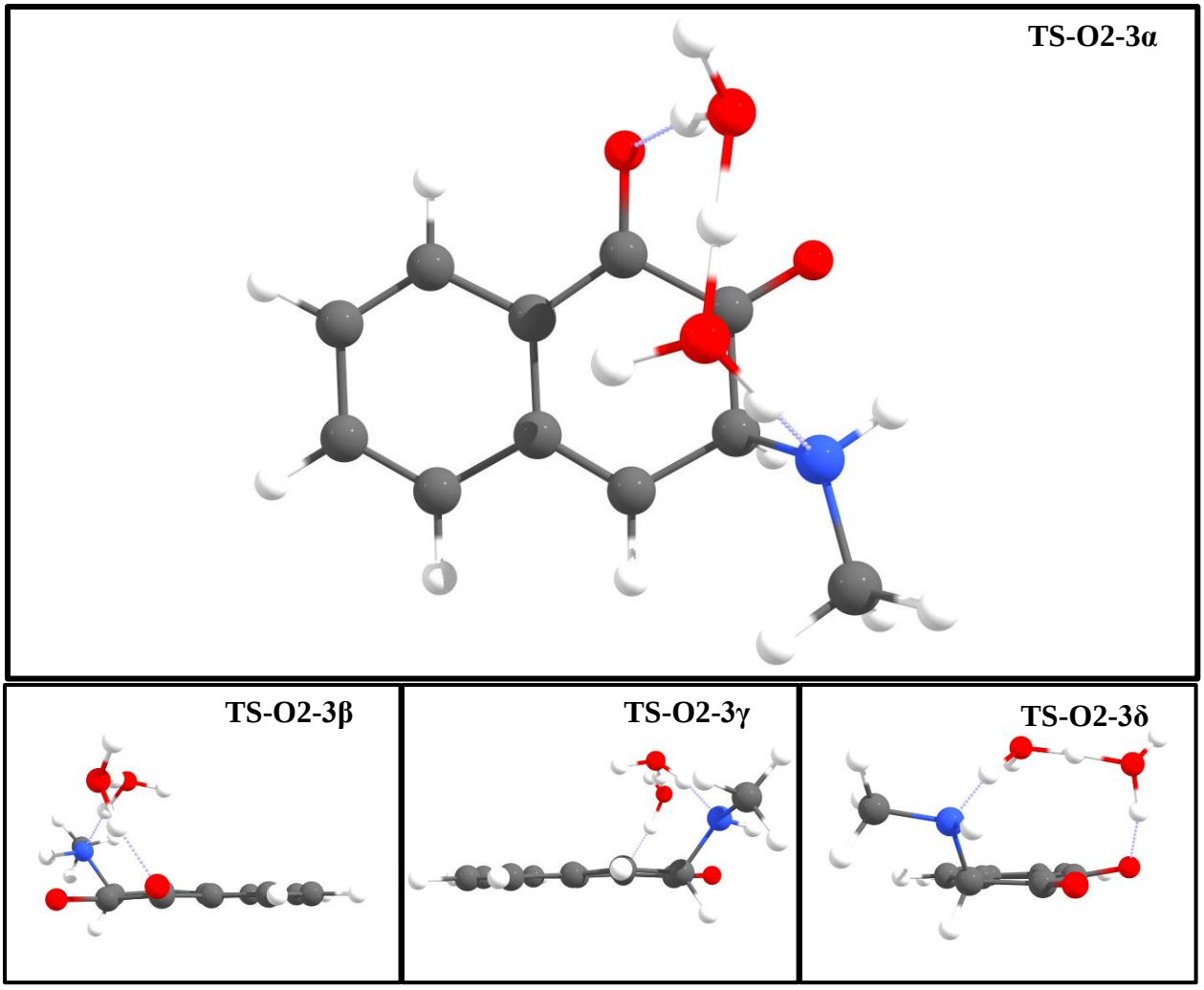


Figure 4.21 Transition state **TS-O2-3**: Third lowest energy structure for **R-O2** reaction

As shown in Table 4.4, the intermolecular distances C_3–N_a, O_w–H_w, O_x–H_x, and C_1–O_1 have fairly consistent values around 1.493 Å, 1.171 Å, 1.057 Å, and 1.268 Å, respectively. The transition state **TS-O2-6** was not included in this transition state because it has a completely different structure compared to the other transition state. The remaining intermolecular distances shown in Table 4.4 have enough variation that there does not appear to be a trend.

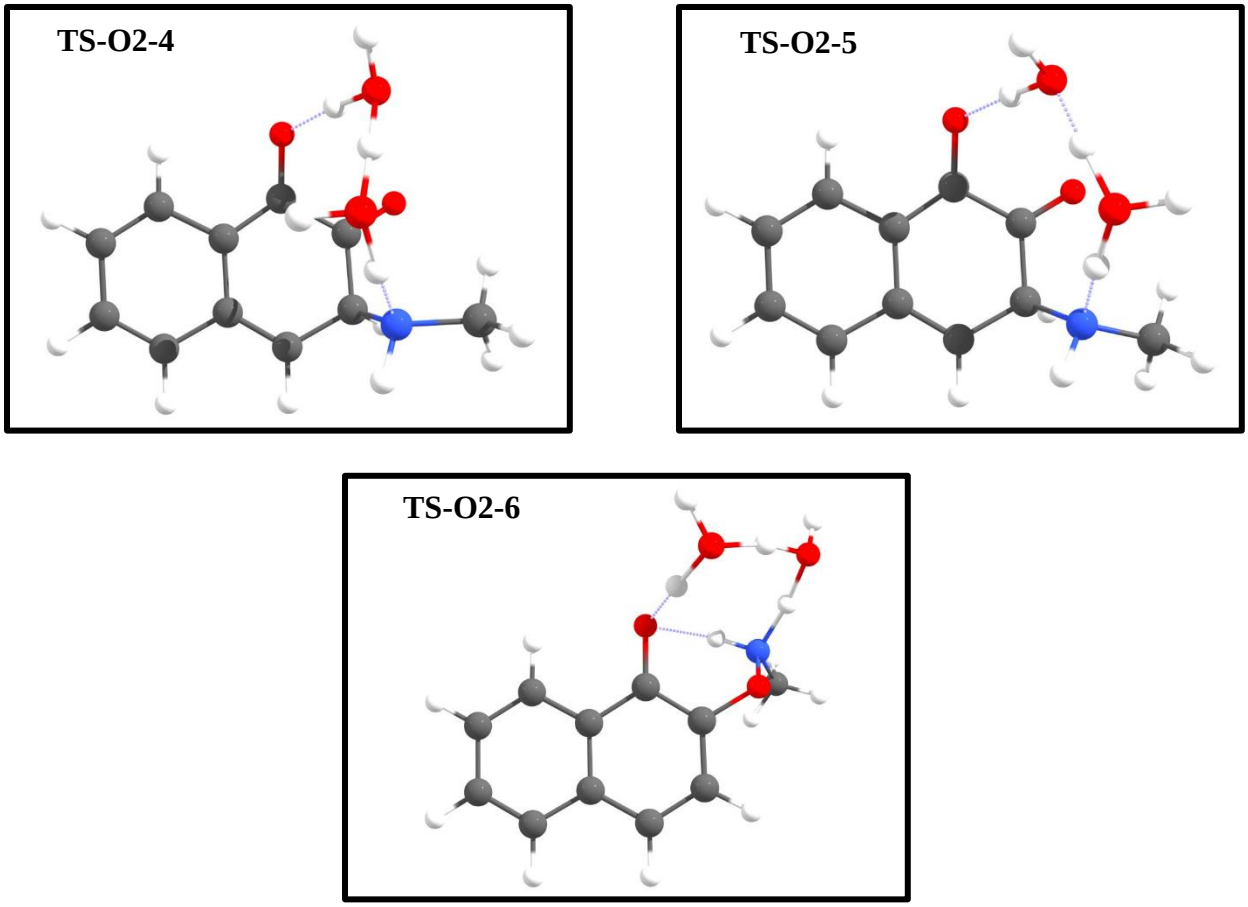


Figure 4.22 Transition states for reaction **R-O2** (energy ranking order 4-6)

4.4.3 1,2-Addition at carbonyl 2 of 1,2-naphthoquinone

Ten different conformers of the transition state were examined, and only seven distinct transition states were identified for the **R-O3** reaction. A summary of some important parameters of the transition states are given in Tables 4.5 and 4.6.

TS-O3-1, **TS-O3-2**, and **TS-O3-3** were the three lowest energy structures optimized for the transition state of the **R-O3** reaction and are shown in Figures 4.23, 4.24, and 4.25. The front views of the remaining optimized transition states are depicted in Figure 4.26.

Table 4.5 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-O3**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-O3-1	0.70	763*i*
TS-O3-2	0.82	705*i*
TS-O3-3	0.93	705*i*
TS-O3-4	2.73	547*i*
TS-O3-5	3.63	574*i*
TS-O3-6	6.91	1423*i*
TS-O3-7	7.08	1320*i*

Table 4.6 Selected internuclear distances (Å) for transition state of reaction **R-O3**

Transition State	C_2—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_2—H_x	C_2—O_2
TS-O3-1	1.506	1.089	1.493	1.134	1.261	1.320	1.097	1.353
TS-O3-2	1.507	1.087	1.494	1.128	1.275	1.339	1.089	1.354
TS-O3-3	1.508	1.089	1.481	1.126	1.275	1.334	1.093	1.353
TS-O3-4	1.515	1.079	1.525	1.133	1.269	1.419	1.051	1.358
TS-O3-5	1.515	1.081	1.510	1.136	1.262	1.439	1.048	1.358
TS-O3-6	1.512	1.189	1.307	1.164	1.226	1.190	1.205	1.343
TS-O3-7	1.560	1.137	1.377	1.193	1.198	1.189	1.208	1.318

As seen in Table 4.5, the transition state **TS-O3-1** was the lowest gas-phase barrier height of 0.70 kcal/mol when compared to that of the reactants. The next two transition states **TS-O3-2** and **TS-O3-3** had gas-phase barrier heights of 0.82 kcal/mol and 0.93 kcal/mol which only have a less than 1 kcal/mol difference to the **TS-O3-1**. The remaining transition states in Table 4.5 are all greater in energy by 2 kcal/mol with **TS-O3-7** having the highest gas-phase barrier at 7.08 kcal/mol. In addition, as seen in Table 4.5, there are two sets of imaginary frequencies that were

observed. The first set includes transition states **TS-O-3** to **5** with imaginary frequencies ranging from 547*i* cm^{-1} to 763*i* cm^{-1}. The second set includes transition states **TS-O1-6** to **7** with imaginary frequencies around 1400*i* cm^{-1}.

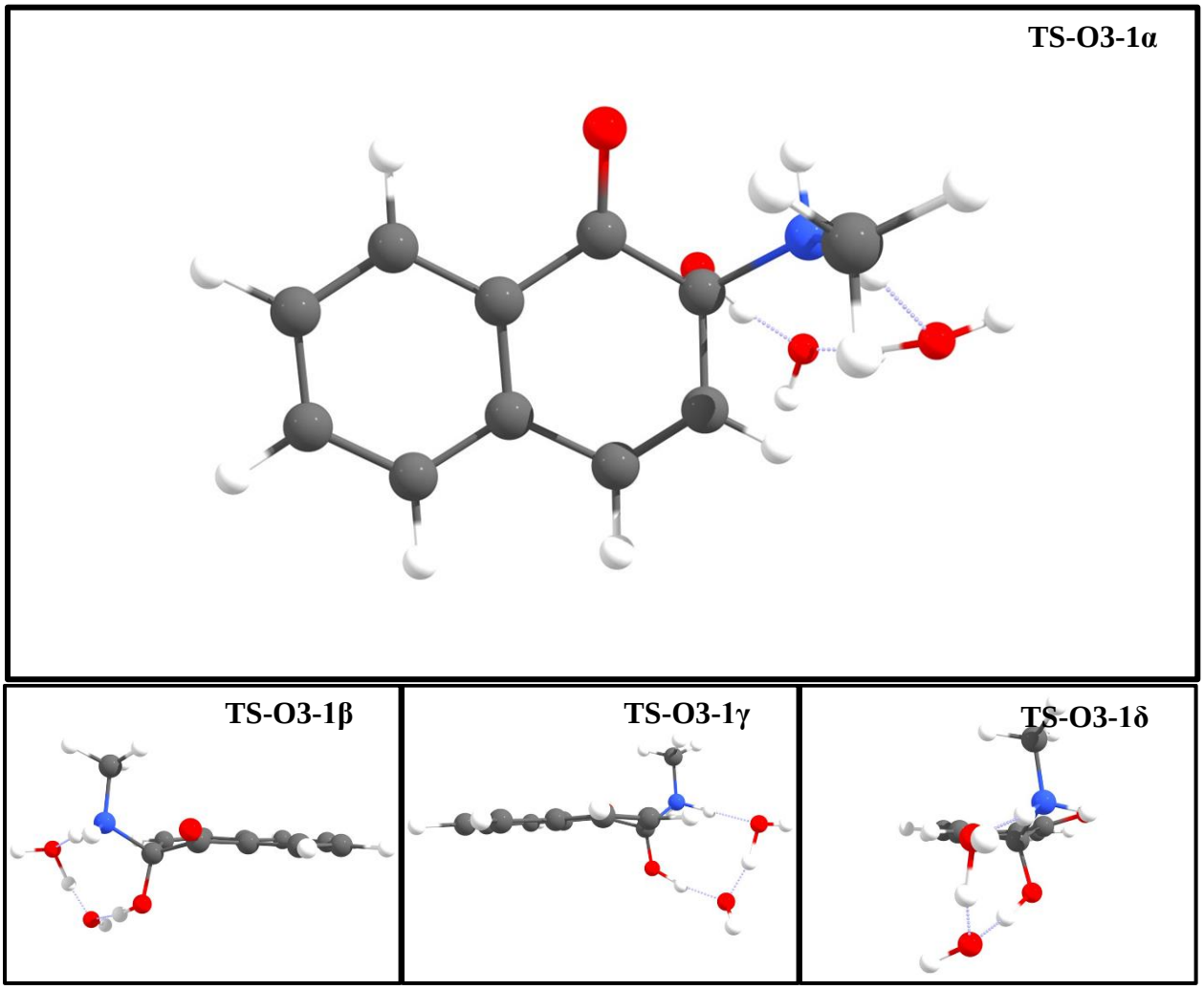


Figure 4.23 Transition state **TS-O3-1**: Lowest energy structure for **R-O3** reaction

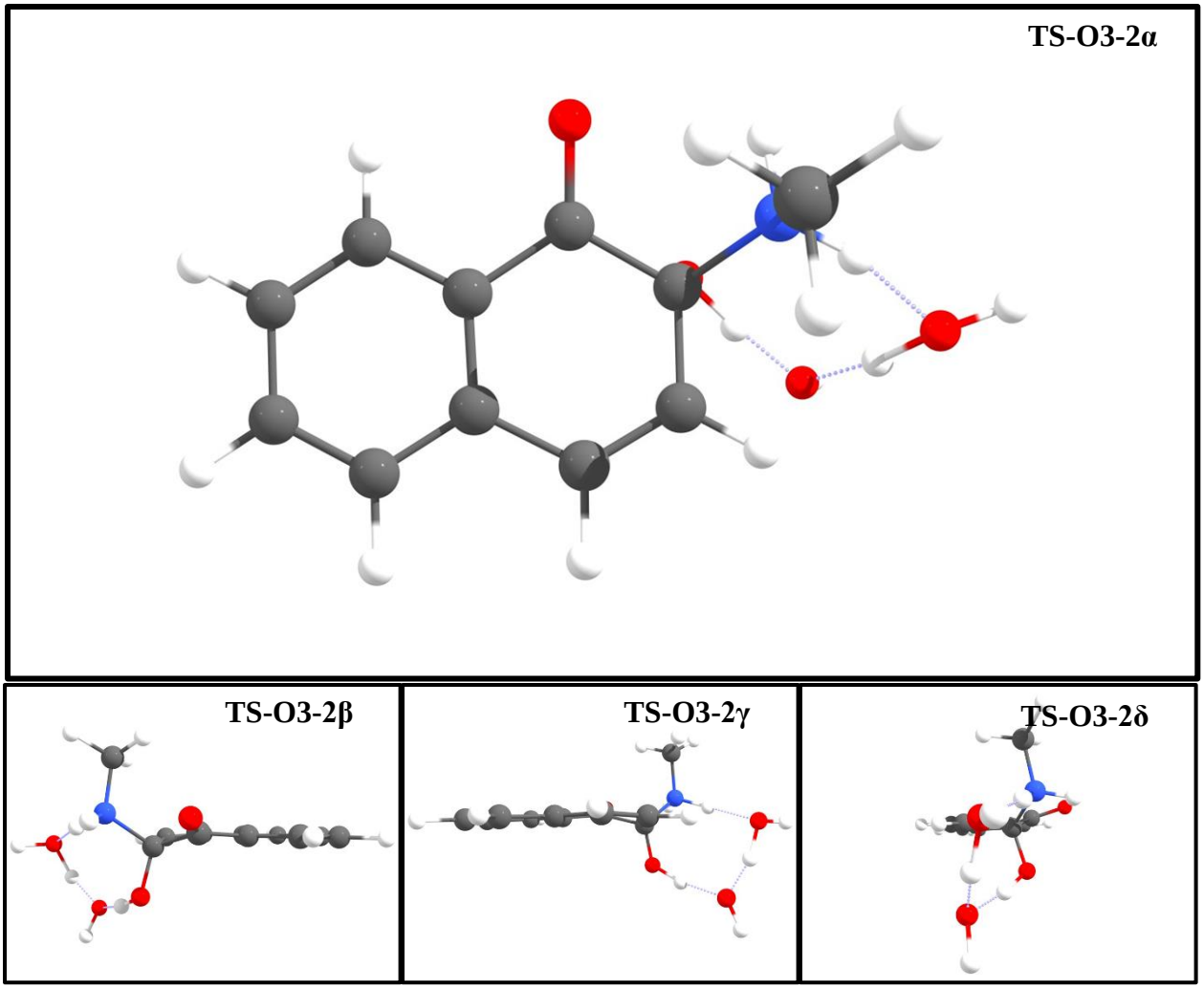


Figure 4.24 Transition state **TS-O3-2**: Second lowest energy structure for **R-O3** reaction

For the intermolecular distances shown in Table 4.6, there would be no trend if transition state **TS-O3-7** is included, so it will be considered an outlier. The intermolecular distances C_2–N_a, N_a–H_a, O_w–H_w, O_2–H_x, and C_2–O_2 for the remaining transition states have fairly consistent values around 1.511 Å, 1.102 Å, 1.137 Å, 1.097 Å, and 1.353 Å, respectively.

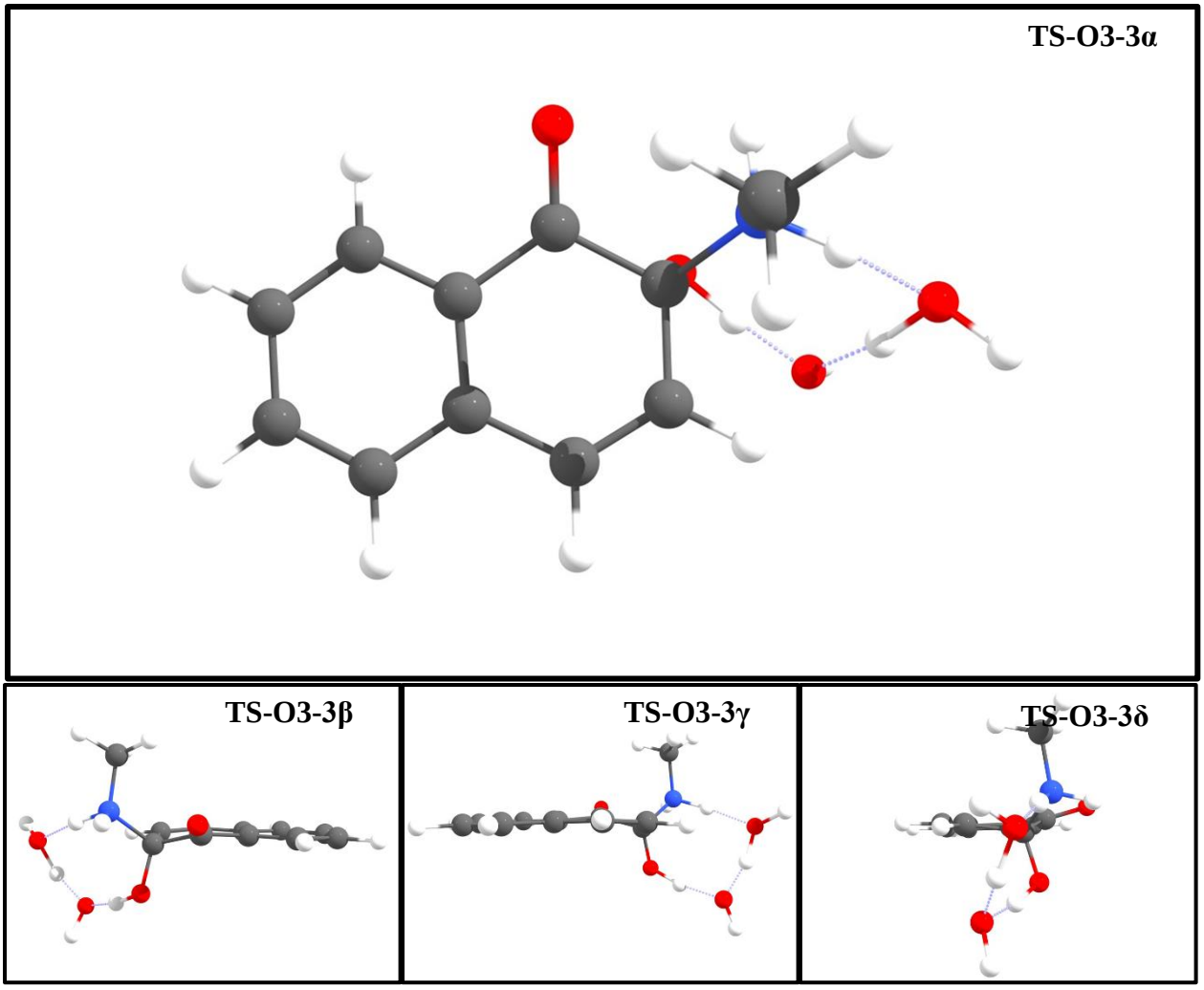


Figure 4.25 Transition state **TS-O3-3**: Third lowest energy structure for **R-O3** reaction

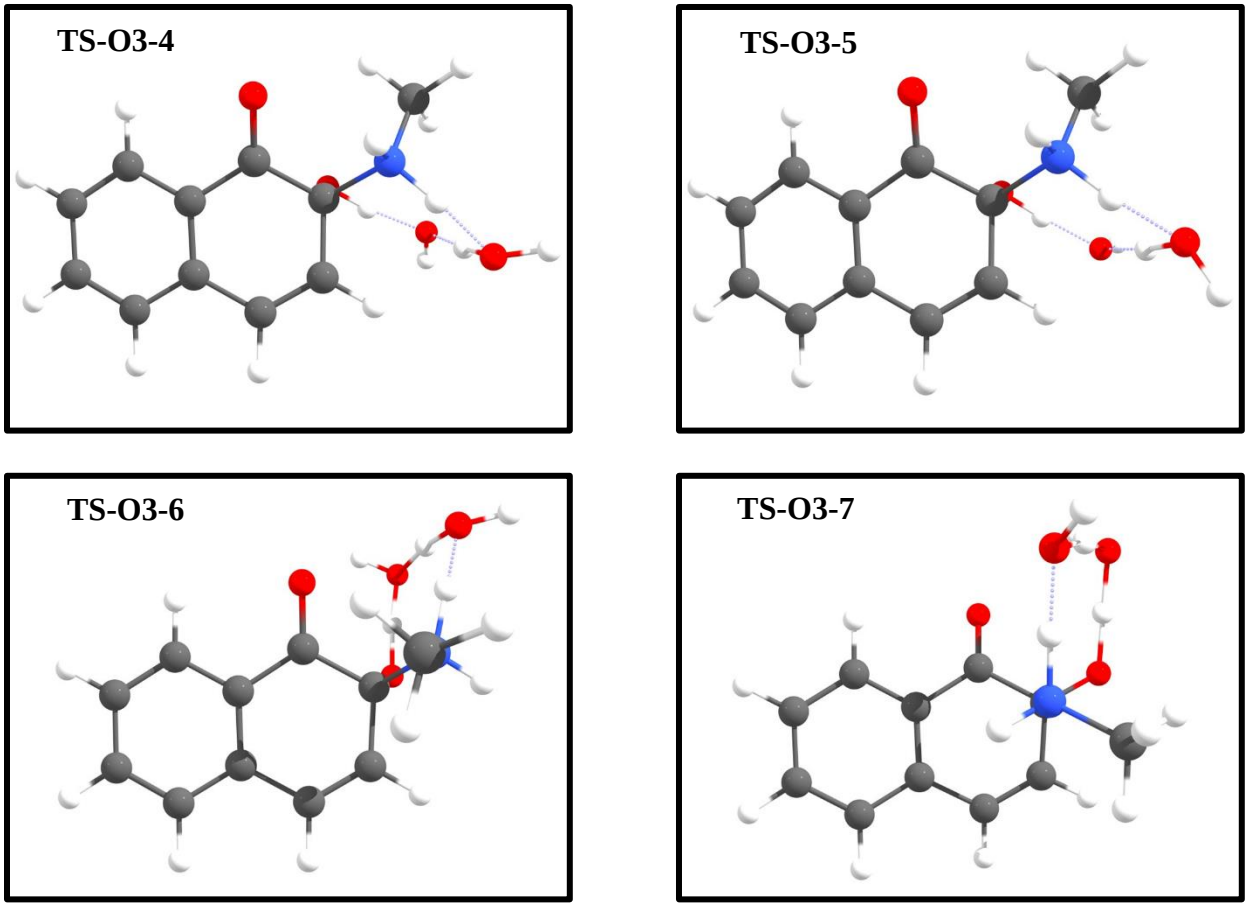


Figure 4.26 Transition states for reaction **R-O3** (energy ranking order 4-7)

4.4.4 1,4-Addition at carbonyl 2 of 1,2-naphthoquinone

Eight different conformers of the transition state were examined, and only five distinct transition states were identified for the **R-O4** reaction. A summary of some important parameters of the transition states are given in Tables 4.7 and 4.8.

TS-O4-1 and **TS-O4-2** the two lowest energy structures optimized for the transition state of the **R-O4** reaction and are shown in Figures 4.27 and 4.28. The front views of the remaining optimized transition states are depicted in Figure 4.29.

Table 4.7 Gas-phase barrier heights (kcal/mol) and imaginary frequencies (cm^{-1}) for transition states of reaction **R-O4**

Transition State	$V^{\ddagger}$ (kcal/mol)	$\omega^{\ddagger}$ (cm^{-1})
TS-O4-1	7.73	989*i*
TS-O4-2	8.72	655*i*
TS-O4-3	10.23	1073*i*
TS-O4-4	10.53	1360*i*
TS-O4-5	12.09	1425*i*

Table 4.8 Selected internuclear distances (Å) for transition state of reaction **R-O4**

Transition State	C_4—N_a	N_a—H_a	O_w—H_a	O_w—H_w	O_x—H_w	O_x—H_x	O_2—H_x	C_2—O_2
TS-O4-1	1.522	1.103	1.456	1.112	1.304	1.247	1.154	1.287
TS-O4-2	1.516	1.099	1.476	1.092	1.342	1.319	1.108	1.297
TS-O4-3	1.517	1.124	1.415	1.117	1.288	1.227	1.163	1.289
TS-O4-4	1.512	1.207	1.284	1.213	1.192	1.104	1.322	1.280
TS-O4-5	1.511	1.218	1.271	1.185	1.210	1.129	1.282	1.284

As seen in Table 4.7, the transition state **TS-O4-1** was the lowest gas-phase barrier height of 7.73 kcal/mol when compared to that of the reactants. The second lowest transition states **TS-O4-2** has a gas-phase barrier height of 8.72 kcal/mol which is only a 1 kcal/mol difference to the transition state **TS-O4-1**. The remaining transition states in Table 4.7 are all greater in energy by 2.5 kcal/mol with **TS-O3-5** having the highest gas-phase barrier at 12.09 kcal/mol. In addition, as seen in Table 4.7, there is a large range for the imaginary frequencies that were observed. The imaginary frequencies for the transition states ranged from 655*i* cm^{-1} to 1425*i* cm^{-1}.

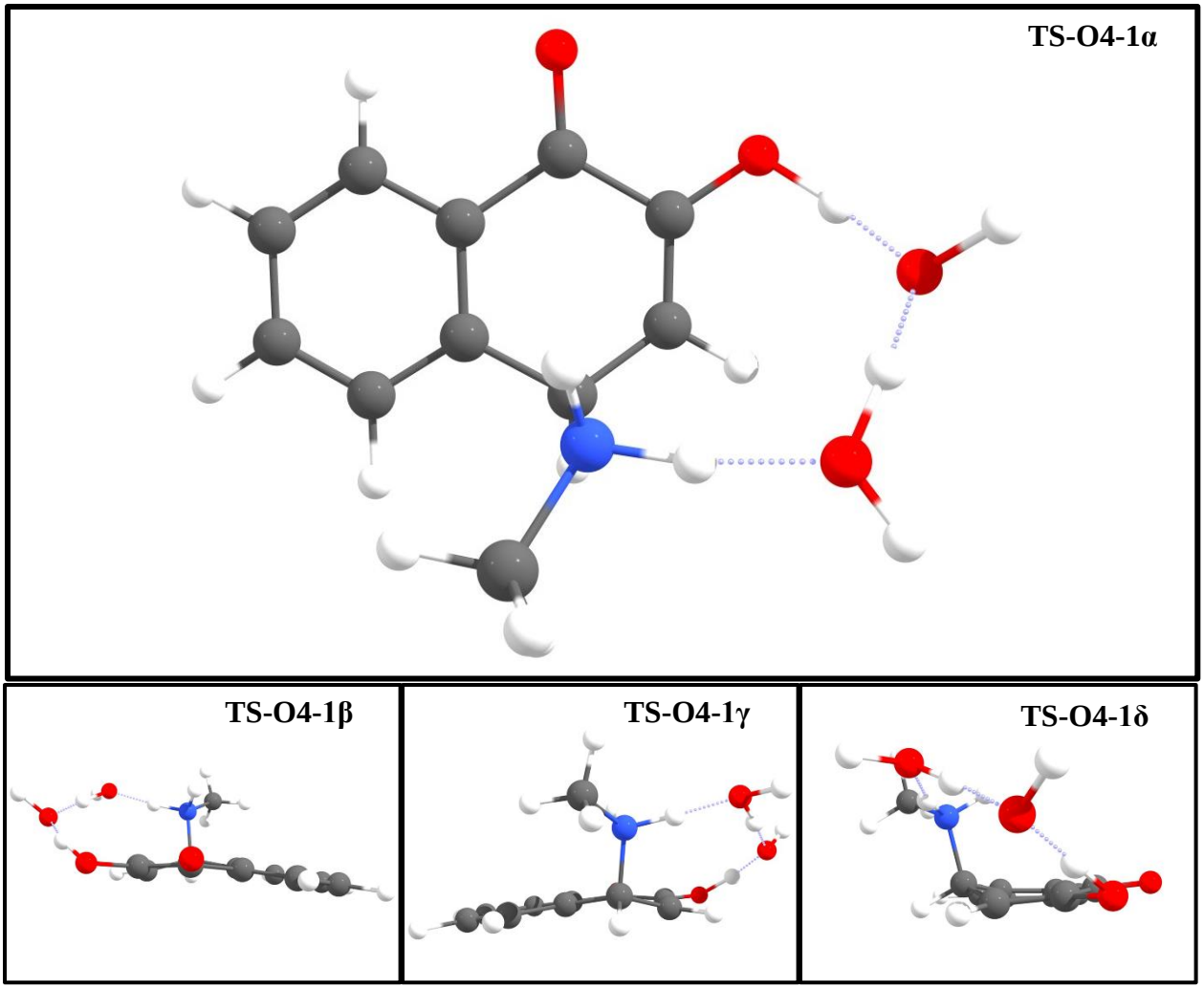


Figure 4.27 Transition state **TS-O4-1**: Lowest energy structure for **R-O4** reaction

As shown in Table 4.8, intermolecular distances C_4–N_a and C_1–O_1 have fairly consistent values around 1.516 Å and 1.287 Å, respectively. The remaining intermolecular distances have enough variation to not have a trend.

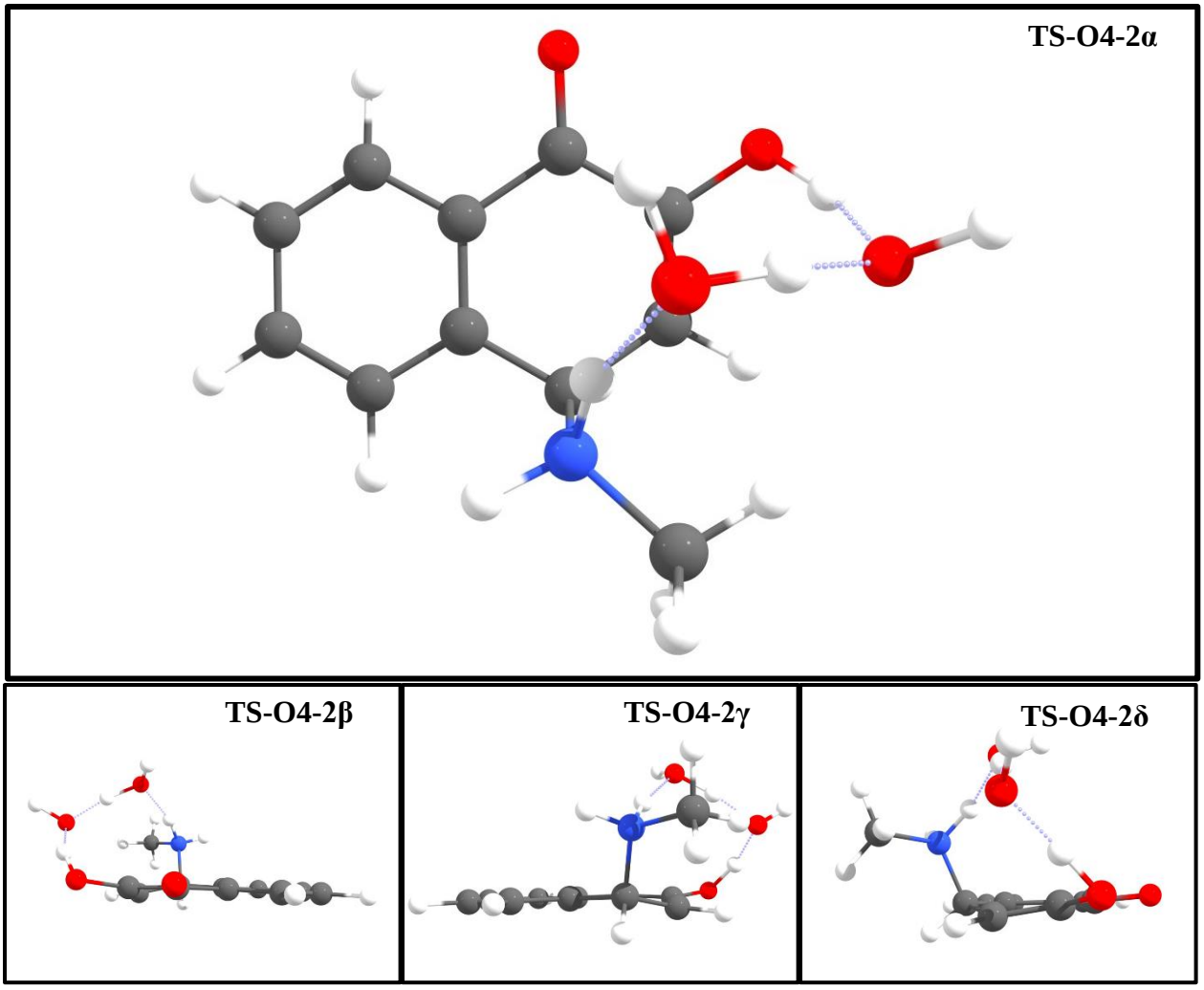


Figure 4.28 Transition state **TS-O4-2**: Second lowest energy structure for **R-O4** reaction

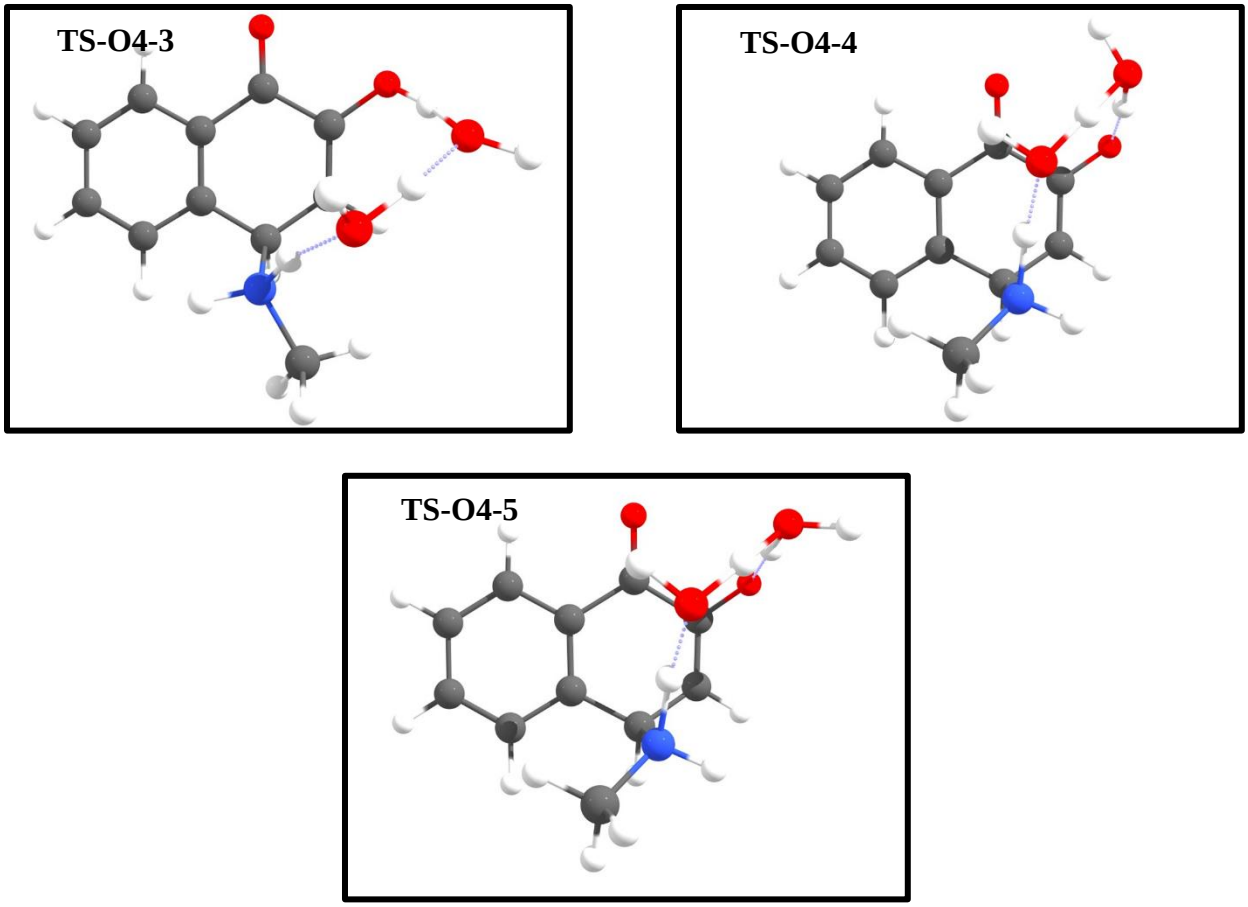


Figure 4.29 Transition states for reaction **R-O4** (energy ranking order 3-5)

4.5 Energy diagram for the reaction between ONQ and methylamine

Once again, each reaction pathway has reactants, reactant complexes, transition states, and products that must be examined to understand the overall reactivity of the naphthoquinone toward the amino group of methylamine. As a result, all the individual stages of the reaction pathway 1,2-naphthoquinone and methylamine has been investigated. Now, it is necessary to take into consideration the information from each section that examined the individual stages.

The lowest gas-phase barrier height structure of 1,2-naphthoquinone and the two water molecules with methylamine as a trimer in section 2.2 were utilized to represent the energy of the reactants. In addition, the energy of the reactants was used as a reference (i.e., having a value of 0.00 kcal/mol), and all other structures have energy values relative to it. Next, the transition states were examined for each possible reaction pathway. The lowest gas-phase barrier heights of the transition states for the **R-O1**, **R-O2**, **R-O3**, and **R-O4** reactions are 1.08 kcal/mol, 25.01 kcal/mol, 0.70 kcal/mol, and 7.73 kcal/mol, respectively. From these values, the **R-O3** reaction, 1,2-addition at carbonyl 2, is the most likely pathway for the reaction to occur. However, the **R-O1** reaction was only 0.38 kcal/mol higher in energy than the **R-O3** reaction and is also likely to occur. This should be kept in mind but will not be used to build the minimum-energy pathway. After determining this, one will take the lowest gas-phase barrier height of the products for the **R-O3** reaction and the water dimer calculated in section 2.3 to represent the energy of the products in the overall reaction pathway. The relative energy of the products to the reactants was determined to be -4.53 kcal/mol. Another stage examined in the reaction pathway was the reactant complex. The lowest energy structure for the reactant complexes was determined to be -10.18 kcal/mol relative to the reactants. From this value, the difference between the transition

state for the **R-O3** reaction and the reactant complex can be calculated. The relative energy difference is 10.88 kcal/mol and would give a more accurate representation of the barrier height for the reaction occurring in solution. Using this information, the energy diagram of the reaction was constructed and is shown in Figure 4.30.

The product **P-O3-1**, which is represented in Figure 2.43, is 0.87 kcal/mol higher in energy than product **P-O1-1**, 18.56 kcal/mol lower in energy than product **P-O2-1**, and 3.30 kcal/mol higher in energy than product **P-O4-1**. Although it is not the most likely product based on the transition states, these energy values presented here suggest that the product **P-O4-1** is the lowest energy product and is the most stable product.

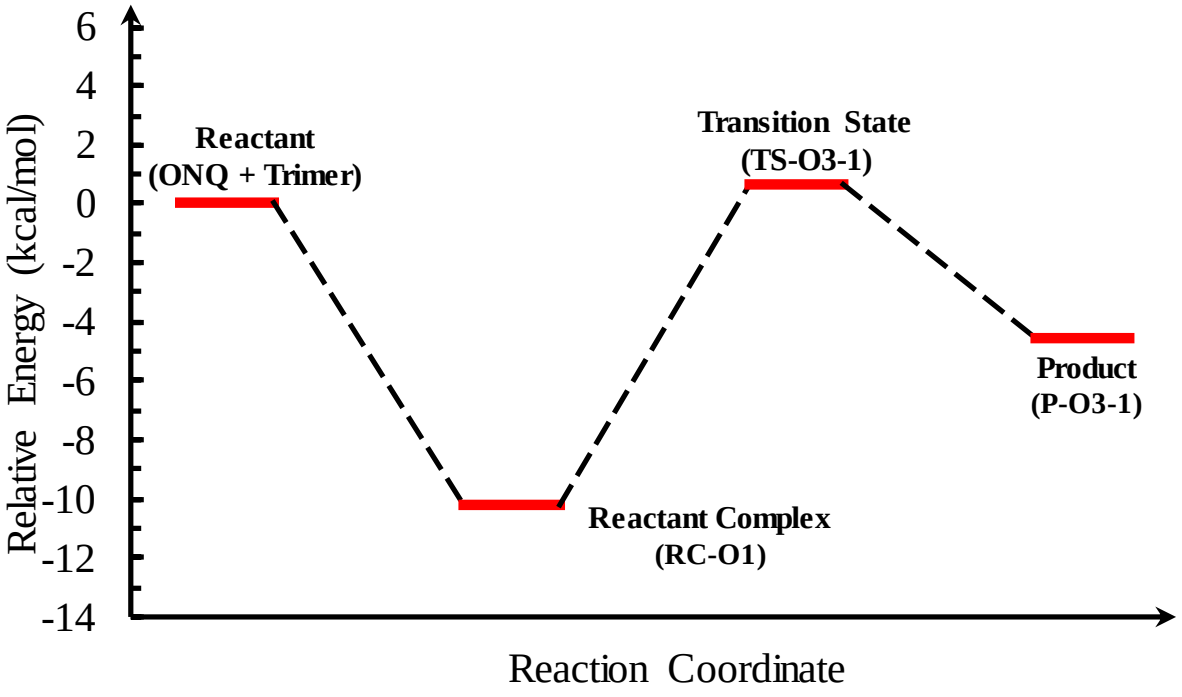


Figure 4.30 Energy diagram for the reaction between 1,2-naphthoquinone and methylamine in the presence of two water molecules

CHAPTER 5

COMPARISON OF NAPHTHOQUINONES

5.1 Introduction

In the previous three chapters, the reaction pathways for the reactions of different naphthoquinones with methylamine were determined by examining the reactants, reactant complexes, transition states, and products in each reaction pathway. By determining the relative energies of various reaction stages, one can assess the overall reactivity of each naphthoquinone toward an amino group and use these reactivities to compare the naphthoquinones against one another. The reaction energy diagrams for the reaction of 2-hydroxy-1,4-naphthoquinone, 1,4-naphthoquinone, and 1,2-naphthoquinone with methylamine can be seen in Figures 2.43, 3.18, and 4.30, respectively. The reaction pathways characterize the theoretically determined reactivity of each naphthoquinone, and these calculations of the naphthoquinone reactivity can be compared with the experimental results obtained by Charles Thomas using fluorescence and UV-Vis spectroscopy and Neethu Kurien using the SDS-PAGE technique. Both of these experimental studies on naphthoquinone reactivity toward Lysozyme, an amyloidal protein, showed that the reactivity of ONQ was the greatest, followed by PNQ, and lastly HNQ [Thomas Jr., 2017; Kurien, 2018]. By comparing our theoretically determined values with the experimental results for the naphthoquinone reactivity, we can assess how well our model replicates what is occurring in solution. A direct comparison of the naphthoquinone reactivities presented in the previous chapters will be conducted here, and these results will be further compared with experimentally determined results.

5.2 Reactivity of naphthoquinones

To start the comparison between naphthoquinones, one will need to examine the reaction path of each naphthoquinone reacting with methylamine. Figures 2.43, 3.18, and 4.30 depict the reaction pathway of HNQ, PNQ, and ONQ, respectively, reacting with methylamine in the presence of two water molecules. To assess the reactivity, one will have to focus on the energy difference between the transition states and the reactants namely the barrier height (less accurately described as activation energy) that represents the energy barrier required for the reactants in order to transform into the products. As a first approach, the reactants are considered to be the naphthoquinone and the trimer of two water molecules and methylamine. The gas-phase barrier heights for HNQ, PNQ, and ONQ are 4.50 kcal/mol, 7.97 kcal/mol, and 1.07 kcal/mol, respectively. Based on of these energy values, ONQ is predicted to be the most reactive, followed by HNQ, and lastly PNQ. However, this prediction is not totally consistent with what was observed experimentally where ONQ was found to be the most reactive, followed by PNQ, and lastly HNQ. ONQ has the highest reactivity both theoretically and experimentally, but PNQ and HNQ have been swapped in reactivity. This means that the model for the reaction pathway that starts from the separated reactants might not accurately depict what is occurring in solution, so we attempted to improve the model by examining reactant complexes as a starting point of the reaction.

As a second approach to determine relative reactivities of the naphthoquinones, reactant complexes were also considered as the starting point of the reaction. As seen in Figures 2.43, 3.18, and 4.30, the gas-phase barrier height of the transition states relative to the reactant complexes for HNQ, PNQ, and ONQ are 13.64 kcal/mol, 14.16 kcal/mol, and 10.88 kcal/mol, respectively. Once again, the reactivity for each naphthoquinone would still be highest for ONQ,

followed by HNQ, and lastly PNQ with these new values for barrier heights. Once again, the relative reactivities of HNQ and PNQ are still switched, but it is interesting to note that the energy difference between them has been reduced to about 0.5 kcal/mol. This small energy difference would suggest that both naphthoquinones are almost equal in reactivity when considering the transition states relative to the reactant complexes. This result is still not totally consistent with experimentally determined results that show that PNQ is more reactive than HNQ. Although our model is not totally consistent with the experimental results it could get better if additional interactions that can occur in solution would be added to the model, and future research will be necessary to build such more accurate model.

5.3 Concluding remarks

In this study, reactivity of three naphthoquinones, 2-hydroxy-1,4-naphthoquinone, 1,4-naphthoquinone, and 1,2-naphthoquinone, with an N-containing nucleophile, methylamine, were theoretically investigated. The studied nucleophilic additions were taken place at several different positions on the naphthoquinone ring, namely carbonyl 1, 2, or 4. The hybrid density functional method mPW1B95-44 in conjunction with basis set 6-31+G(d,p) was used during the study for all the electronic structure calculations on *Gaussian 09* software. All of the computations were carried out in gas-phase.

Detailed conformation analyses were carried out for the reactants, reactant complexes, and products for each of the possible reaction pathways, for each naphthoquinone. In addition, the transition states were also examined to determine the minimum-energy barrier height for the reactions occurring for each naphthoquinone. These transition states were examined by modeling

the hydrogen transfer with the assistance of two water molecules, and each investigated reaction takes place through at least two different pathways. HNQ, PNQ, and ONQ had 4, 2, and 4 possible pathways, respectively. For the HNQ reaction, the lowest gas-phase transition state was found for the 1,2-addition at carbonyl 1 with an energy of 4.50 kcal/mol relative to the reactants. For the PNQ reaction, the lowest gas-phase transition state was found for the 1,4-addition with an energy of 7.97 kcal/mol relative to the reactants. Lastly, for the ONQ reaction, the lowest gas-phase transition state was found for the 1,2-addition at carbonyl 2 with an energy of just 0.70 kcal/mol relative to the reactants. Overall, all of these transition states were determined to have an imaginary frequency and have some consistency in their intermolecular distances.

It was observed that the separated products for HNQ and PNQ have a positive energy relative to the reactants which make the reactions less likely experimentally, since the reactions are endothermic. Only ONQ has a negative value for its products, and it is only slightly negative. This difference might be due to the fact that the energy of a water dimer was just added to the product energy. This does not consider the interactions that might occur if the two water molecules were in a trimer with the product, and like the reactant complexes, these interactions should lower the energy of the products considerably. Therefore, if one wanted to build a more accurate reaction pathway, one would have to examine the possibility and the energies of the product complexes.

After comparing the theoretical values calculated for each naphthoquinone, it was determined that ONQ was the most reactive, followed by HNQ, and PNQ as the least reactive. However, this ranking is not totally consistent with the experimentally determined reactivities that shown that PNQ being more reactive than HNQ. More work must be done to include

possible interactions that either lower the reactivity of HNQ or make PNQ more reactive in our current model to have a better correlation with the experimental observations.

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APPENDIX A

SUPPLEMENTARY INFORMATION FOR CHAPTER 2, 3, AND 4

This appendix includes the optimized geometries in Cartesian coordinates for minimum-energy structures and transition states in gas-phase using the mPW1B95-44/6-31+G(d,p) level of theory.

Cartesian coordinates of reactants

RE-H1

C	0.000000	-0.803088	0.000000
C	0.974608	0.192194	0.000000
C	2.311472	-0.160638	0.000000
C	2.670179	-1.497724	0.000000
C	1.697845	-2.487159	0.000000
C	0.359496	-2.141889	0.000000
H	3.049724	0.625768	0.000000
H	3.713889	-1.771534	0.000000
H	1.985875	-3.526696	0.000000
H	-0.417571	-2.890152	0.000000
C	-1.413566	-0.426208	0.000000
C	-1.757355	1.021249	0.000000
C	-0.818356	1.975082	0.000000
C	0.596763	1.633491	0.000000
H	-1.076831	3.021307	0.000000
O	-2.332865	-1.219064	0.000000
O	-3.055747	1.265462	0.000000
O	1.453710	2.491349	0.000000
H	-3.502388	0.407466	0.000000

RE-H2

C	0.000000	-0.807571	0.000000
C	0.976444	0.184119	0.000000
C	2.315794	-0.164841	0.000000
C	2.677759	-1.499714	0.000000
C	1.704297	-2.488332	0.000000
C	0.365531	-2.144478	0.000000
H	3.051692	0.623855	0.000000
H	3.721662	-1.772669	0.000000
H	1.992137	-3.528083	0.000000
H	-0.411091	-2.893110	0.000000
C	-1.433429	-0.457713	0.000000
C	-1.773743	0.996333	0.000000
C	-0.825195	1.942619	0.000000
C	0.595103	1.617799	0.000000
H	-1.069053	2.995152	0.000000
O	-2.308578	-1.285756	0.000000
O	-3.082100	1.213606	0.000000
O	1.436478	2.491292	0.000000
H	-3.267117	2.152386	0.000000

RE-H3

C	0.000000	-0.839951	0.000000
C	0.875211	0.247731	0.000000
C	2.243522	0.025703	0.000000
C	2.731884	-1.269996	0.000000
C	1.863224	-2.348688	0.000000
C	0.497119	-2.131304	0.000000
H	2.916832	0.866789	0.000000
H	3.797862	-1.436466	0.000000
H	2.249861	-3.355703	0.000000
H	-0.206869	-2.948901	0.000000
C	-1.461993	-0.625522	0.000000
C	-1.972289	0.824828	0.000000
C	-0.982972	1.877324	0.000000
C	0.334369	1.606057	0.000000
H	-1.350614	2.892895	0.000000
O	-2.247823	-1.534001	0.000000
O	-3.161175	1.028272	0.000000
O	1.277109	2.551103	0.000000
H	0.879593	3.421302	0.000000

RE-H4

C	-0.368587	0.739570	-0.021887
C	-0.669273	-0.625476	0.000272
C	-2.001870	-1.009610	0.048162
C	-3.011216	-0.061021	0.046663
C	-2.704605	1.287133	0.007434
C	-1.379756	1.682720	-0.021927
H	-2.292442	-2.048903	0.103474
H	-4.040354	-0.382223	0.082939
H	-3.492522	2.023448	0.006737
H	-1.099964	2.724583	-0.040914
C	1.037379	1.202879	-0.024483
C	2.139730	0.138051	0.034062
C	1.725779	-1.243827	0.011439
C	0.430207	-1.599254	-0.020754
H	2.492421	-2.000967	0.004338
O	1.324302	2.368416	-0.063641
O	3.292014	0.492632	0.078217
O	0.138015	-2.902102	-0.050797
H	-0.788515	-3.054501	-0.220688

T-a

N	-1.028776	0.080604	-0.583379
H	-1.410996	0.085729	-1.515095
C	-2.082481	0.172529	0.409547
H	-0.395182	0.866357	-0.510995
H	0.287249	-1.134949	-0.165189
O	1.146367	-1.463552	0.172038
O	1.700875	1.245725	0.002890
H	1.790331	0.292513	0.136067
H	2.289396	1.672149	0.617981
H	1.427035	-2.174517	-0.396254
H	-2.701639	1.067135	0.322463
H	-1.637718	0.165779	1.400408
H	-2.730093	-0.696979	0.337558

T-b

N	-1.029046	0.014336	0.571594
C	-2.097419	0.175025	-0.395932
H	-1.397799	-0.070442	1.504937
H	-0.409500	0.814422	0.559311
H	0.344950	-1.154390	0.187926
O	1.255805	-1.452031	-0.015118
O	1.615667	1.291723	-0.126168
H	1.769575	0.338663	-0.174410
H	2.434818	1.694520	0.144630
H	1.201448	-2.098507	-0.712398
H	-2.735428	1.042429	-0.217790
H	-2.725785	-0.711741	-0.399729
H	-1.666223	0.277008	-1.387749

T-b

H	-0.309367	-1.211056	0.179986
N	1.093263	-0.134612	0.687067
H	1.743074	-0.369018	1.419733
H	0.527493	0.637641	1.009104
O	-1.177680	-1.409211	-0.228039
H	-1.546263	-2.156120	0.232930
H	-1.602025	0.397980	-0.119393
O	-1.430330	1.337912	0.031421
H	-2.234403	1.805665	-0.171510
C	1.791090	0.238692	-0.531471
H	2.486203	1.070298	-0.406965
H	1.056859	0.521458	-1.279582
H	2.343125	-0.616331	-0.912007

RE-P1

C	0.486606	-0.562968	0.000000
C	0.000000	0.742775	0.000000
C	0.882066	1.811153	0.000000
C	2.244185	1.576331	0.000000
C	2.728940	0.275844	0.000000
C	1.852858	-0.793369	0.000000
H	0.479947	2.812134	0.000000
H	2.932787	2.406955	0.000000
H	3.793137	0.098049	0.000000
H	2.203760	-1.813478	0.000000
C	-0.447152	-1.710681	0.000000
C	-1.891130	-1.413593	0.000000
C	-2.355484	-0.166237	0.000000
C	-1.456788	1.001598	0.000000
H	-3.411306	0.058128	0.000000
O	-0.056117	-2.856255	0.000000
O	-1.908785	2.124564	0.000000
H	-2.543711	-2.273372	0.000000

RE-O1

C	0.000000	0.597220	0.000000
C	1.070729	-0.302477	0.000000
C	2.366202	0.195923	0.000000
C	2.591736	1.561929	0.000000
C	1.525966	2.446991	0.000000
C	0.229925	1.961972	0.000000
H	3.199716	-0.490625	0.000000
H	3.603798	1.936011	0.000000
H	1.705772	3.510475	0.000000
H	-0.620964	2.625480	0.000000
C	-1.386282	0.091316	0.000000
C	-1.591166	-1.434126	0.000000
C	-0.397593	-2.274904	0.000000
C	0.825590	-1.736034	0.000000
H	-0.556577	-3.341647	0.000000
O	-2.345287	0.815849	0.000000
O	-2.709348	-1.879296	0.000000
H	1.694692	-2.378974	0.000000

Cartesian coordinates of reactant complexes

RC-H1

C	1.325377	0.606987	-0.099589
C	2.600355	0.058417	-0.002468
C	3.709413	0.883630	-0.039586
C	3.546252	2.251204	-0.173937
C	2.275432	2.798554	-0.272440
C	1.164598	1.977401	-0.235326
H	4.685625	0.431352	0.038086
H	4.412034	2.894614	-0.203014
H	2.153890	3.865279	-0.378496
H	0.167440	2.380801	-0.312445
C	0.142342	-0.265675	-0.059331
C	0.354821	-1.734218	0.078054
C	1.596273	-2.244984	0.170556
C	2.781883	-1.412935	0.139478
H	1.742925	-3.307830	0.273009
O	-0.991683	0.158673	-0.133565
O	-0.710657	-2.493005	0.105166
O	3.898298	-1.883446	0.224629
H	-1.569807	-2.014564	0.039936
O	-4.549723	0.022471	-1.474108
H	-4.256226	0.805056	-0.952197
H	-4.320496	0.185490	-2.384546
O	-3.270309	-1.841902	0.017520
H	-3.787160	-2.642652	0.030924
H	-3.716821	-1.225103	-0.591614
N	-3.537224	1.860153	0.284942
H	-3.642097	2.859430	0.217161
H	-2.558835	1.637938	0.172314
C	-4.013888	1.370043	1.568964
H	-5.080884	1.555605	1.654733
H	-3.515741	1.824411	2.426395
H	-3.857824	0.296243	1.611772

RC-H2

C	1.351136	0.625389	0.123214
C	2.573240	0.014259	-0.138632
C	3.716353	0.782510	-0.255579
C	3.639512	2.156943	-0.111049
C	2.421744	2.767207	0.151569
C	1.276692	2.002578	0.271179
H	4.650365	0.282498	-0.458353
H	4.531799	2.756786	-0.202887
H	2.367920	3.838843	0.263751
H	0.319124	2.454007	0.477979
C	0.133816	-0.186672	0.261792
C	0.233631	-1.659157	0.052889
C	1.431897	-2.227817	-0.186618
C	2.656504	-1.463745	-0.296545
H	1.505046	-3.294941	-0.319309
O	-0.941577	0.310010	0.538173
O	-0.854029	-2.374873	0.141369
O	3.727091	-1.993227	-0.516827
H	-1.723064	-1.892244	0.222085
O	-3.307968	-1.564134	0.268729
H	-3.606579	-1.353930	1.153743
H	-3.510149	-0.752548	-0.247107
O	-3.302835	0.662978	2.119598
H	-3.147805	0.989585	3.001481
H	-2.441482	0.564144	1.703203
N	-3.827650	0.911694	-0.876482
H	-4.089731	1.344793	-0.002979
H	-2.939890	1.307110	-1.142856
C	-4.830680	1.120282	-1.902776
H	-5.023928	2.169303	-2.133726
H	-5.765146	0.665442	-1.587306
H	-4.521452	0.622598	-2.817337

RC-H3

C	1.412855	0.580282	0.005887
C	2.494704	-0.293544	-0.035071
C	3.775508	0.203081	-0.187643
C	3.975429	1.568228	-0.300278
C	2.897835	2.440586	-0.257386
C	1.616088	1.948379	-0.100174
H	4.595680	-0.497047	-0.214215
H	4.975264	1.955637	-0.421325
H	3.059640	3.503574	-0.344738
H	0.764311	2.608590	-0.057215
C	0.051514	0.059633	0.189239
C	-0.151101	-1.417283	0.229560
C	0.918725	-2.239918	0.207430
C	2.279213	-1.761889	0.083825
H	0.777839	-3.307031	0.264278
O	-0.906020	0.803109	0.310316
O	-1.368189	-1.866913	0.333604
O	3.228562	-2.519611	0.063749
H	-2.157505	-1.227740	0.133561
O	-3.218874	2.253729	-1.148123
H	-3.424000	2.378969	-0.217128
H	-2.264660	2.249387	-1.184487
O	-3.236991	1.672998	1.647732
H	-3.147079	2.118382	2.485693
H	-2.381410	1.286281	1.436799
N	-3.572398	-0.646524	-0.224717
H	-4.027652	-0.355454	0.628316
H	-3.487160	0.197666	-0.780100
C	-4.367303	-1.647493	-0.919209
H	-5.367906	-1.300939	-1.175281
H	-4.455975	-2.535762	-0.300795
H	-3.861305	-1.935705	-1.835645

RC-H4

C	-1.665713	-0.752397	-0.027791
C	-1.636035	0.590677	0.336090
C	-2.688219	1.416604	-0.011753
C	-3.764051	0.900979	-0.714565
C	-3.791090	-0.437668	-1.075876
C	-2.739657	-1.268008	-0.733963
H	-2.644101	2.455462	0.274665
H	-4.586312	1.545941	-0.983431
H	-4.632368	-0.831830	-1.624257
H	-2.732524	-2.312281	-1.004506
C	-0.549281	-1.619050	0.344310
C	0.555924	-1.036905	1.151948
C	0.574513	0.248928	1.515741
C	-0.480263	1.151337	1.083693
H	1.385475	0.668110	2.089098
O	-0.469274	-2.797243	0.062391
O	1.506537	-1.906455	1.460067
O	-0.425809	2.342716	1.324778
H	1.237079	-2.752057	1.072009
O	0.964325	0.332838	-1.643449
H	1.856839	0.019040	-1.371006
H	0.917433	0.271631	-2.593608
O	2.113525	2.592397	-0.262206
H	1.545925	2.053280	-0.823416
H	1.525302	2.983278	0.382720
N	3.418535	-0.124016	-0.471594
H	3.350369	0.809249	-0.084483
H	3.319991	-0.778124	0.289444
C	4.680773	-0.310141	-1.161122
H	5.558055	-0.194566	-0.522426
H	4.758940	0.412779	-1.968298
H	4.714314	-1.301967	-1.604269

RC-H5

C	1.805413	-0.506499	-0.106193
C	1.388466	0.813298	-0.247067
C	2.247573	1.841472	0.091990
C	3.516200	1.550610	0.564887
C	3.928865	0.234378	0.703576
C	3.072002	-0.798537	0.368366
H	1.903982	2.857699	-0.018277
H	4.186937	2.354092	0.827580
H	4.918331	0.014971	1.073422
H	3.364649	-1.831875	0.469804
C	0.889491	-1.587791	-0.467939
C	-0.439348	-1.223964	-1.035261
C	-0.827325	0.047883	-1.190805
C	0.026956	1.129037	-0.747638
H	-1.796843	0.298682	-1.591728
O	1.152357	-2.768287	-0.380240
O	-1.176772	-2.263751	-1.372483
O	-0.345086	2.293272	-0.790822
H	-0.666221	-3.051125	-1.133517
O	-0.570094	-0.594026	1.860086
H	-1.499732	-0.289050	1.792269
H	-0.375687	-0.671712	2.789413
O	-3.114282	2.342538	-0.725881
H	-3.565289	3.161993	-0.905587
H	-2.166280	2.512294	-0.820504
N	-3.237911	0.206164	1.475713
H	-3.715788	0.535206	2.299792
H	-3.237117	0.974600	0.815222
C	-3.933771	-0.936613	0.910789
H	-4.963536	-0.728400	0.615280
H	-3.942924	-1.752684	1.628734
H	-3.395216	-1.285461	0.034592

RC-H6

C	-1.024033	0.626097	-0.317385
C	-2.143118	-0.185934	-0.166009
C	-3.393596	0.388034	-0.022623
C	-3.525451	1.765269	-0.029287
C	-2.409038	2.574321	-0.184339
C	-1.158115	2.005416	-0.332022
H	-4.244794	-0.265008	0.089873
H	-4.501293	2.212103	0.083151
H	-2.516943	3.647873	-0.191899
H	-0.276965	2.614471	-0.458412
C	0.302273	0.017518	-0.483843
C	0.405498	-1.466839	-0.419872
C	-0.690895	-2.236606	-0.310478
C	-2.013415	-1.670029	-0.162299
H	-0.607022	-3.310937	-0.292110
O	1.299881	0.663131	-0.739583
O	1.610455	-1.980439	-0.488844
O	-3.001303	-2.366036	-0.028529
H	2.320998	-1.323950	-0.640739
O	3.730942	2.000625	-0.589560
H	3.958088	2.618081	-1.279554
H	2.787902	1.825187	-0.668537
O	3.979237	-0.730716	-0.866912
H	4.753857	-1.157490	-0.512958
H	4.096980	0.225808	-0.779522
N	0.837848	-0.251255	2.210498
H	0.188232	0.176162	2.849897
H	0.907800	-1.225857	2.454595
C	2.130221	0.397859	2.245043
H	2.6257420	0.378530	3.218500
H	2.020886	1.436065	1.941980
H	2.785915	-0.075409	1.518364

RC-H7

C	-0.206468	0.909841	-0.626158
C	0.643606	-0.253607	-1.009075
C	0.136896	-1.495331	-1.047681
C	-1.212553	-1.793496	-0.603258
C	-2.045326	-0.667505	-0.104716
C	-1.550654	0.632920	-0.106879
O	0.204187	2.038440	-0.802237
O	-1.649560	-2.926371	-0.619255
H	1.972012	2.843898	-0.615939
N	3.125539	-1.604225	1.212194
H	3.152756	-2.338624	1.900656
H	2.648955	-1.968263	0.402342
O	2.858861	2.494754	-0.484934
H	3.473657	3.085197	-0.912569
H	2.203140	1.443606	1.383559
O	1.571322	0.753934	1.580506
H	2.082014	-0.073760	1.592455
C	4.460885	-1.158123	0.862725
H	4.384845	-0.347726	0.142635
H	5.098627	-1.933830	0.435380
H	4.952033	-0.765121	1.748712
H	0.733119	-2.325577	-1.392042
O	1.881092	-0.001433	-1.387881
H	2.155682	0.897655	-1.142359
C	-2.330269	1.678941	0.360133
C	-3.602921	1.423722	0.834642
C	-4.097421	0.127688	0.836031
C	-3.321504	-0.917127	0.365821
H	-1.921988	2.676913	0.347315
H	-4.211500	2.233757	1.205313
H	-5.092169	-0.067297	1.206079
H	-3.682798	-1.933390	0.354002

RC-H8

C	0.467331	-1.372369	0.308555
C	1.109834	-0.423503	1.264688
C	0.404528	0.554002	1.854760
C	-0.956207	0.850009	1.462028
C	-1.633500	-0.076841	0.517499
C	-0.937201	-1.139312	-0.048958
O	1.098048	-2.324500	-0.100127
O	-1.527028	1.851557	1.855224
H	2.949274	-2.242939	-0.924616
N	1.035951	3.069290	-0.592670
H	0.326735	2.965685	0.117618
H	1.793669	3.578358	-0.165819
O	3.701707	-1.692307	-0.693622
H	4.487491	-2.226725	-0.772281
H	2.647971	0.212771	-1.389453
O	1.710389	0.395974	-1.416115
H	1.580071	1.319263	-1.138219
C	0.509381	3.795712	-1.734857
H	1.285623	3.894560	-2.488320
H	0.132980	4.791939	-1.497081
H	-0.299689	3.223144	-2.178429
H	0.875089	1.223217	2.556753
O	2.379388	-0.626701	1.540677
H	2.798151	-1.198312	0.876130
C	-1.565764	-1.990590	-0.942822
C	-2.892038	-1.779902	-1.270207
C	-3.587364	-0.720218	-0.706438
C	-2.959499	0.132720	0.184268
H	-1.000660	-2.803789	-1.369796
H	-3.385966	-2.439401	-1.966692
H	-4.622899	-0.559289	-0.963993
H	-3.476541	0.966060	0.633482

RC-H9

C	1.750846	0.241345	-0.236155
C	0.961509	-0.888067	-0.433324
C	1.509502	-2.144424	-0.253851
C	2.832600	-2.268918	0.132132
C	3.616340	-1.141947	0.335966
C	3.076755	0.116246	0.149564
H	0.883156	-3.007031	-0.416466
H	3.258309	-3.250365	0.273999
H	4.647182	-1.247857	0.635718
H	3.662669	1.010422	0.294710
C	1.173223	1.567577	-0.446353
C	-0.244104	1.656994	-0.883292
C	-1.002741	0.571142	-1.068541
C	-0.457853	-0.757107	-0.850505
H	-2.033591	0.649628	-1.375616
O	1.779102	2.610201	-0.296102
O	-0.674862	2.895180	-1.059947
O	-1.121687	-1.759500	-1.062849
H	0.070284	3.478577	-0.859368
O	-3.831932	-1.296601	-1.156066
H	-4.366049	-2.047766	-1.397847
H	-2.904310	-1.577201	-1.207489
O	-3.932555	-0.082125	1.349283
H	-4.007279	-0.510287	0.484776
H	-4.462515	0.708164	1.306263
N	-0.927725	-0.313993	1.943472
H	-1.933788	-0.231222	1.872287
H	-0.723838	-1.141462	2.479281
C	-0.348938	0.857522	2.555125
H	-0.677327	1.055359	3.579565
H	-0.603028	1.734693	1.962185
H	0.736857	0.774874	2.564551

RC-H10

C	1.629645	0.042559	-0.533548
C	0.773157	-1.029471	-0.302636
C	1.300851	-2.293666	-0.104880
C	2.671681	-2.481363	-0.135140
C	3.521595	-1.410004	-0.367702
C	3.000813	-0.145257	-0.571236
H	0.621060	-3.112116	0.071281
H	3.080880	-3.467600	0.020710
H	4.589185	-1.563805	-0.393095
H	3.637021	0.705482	-0.759347
C	1.062996	1.375869	-0.746458
C	-0.416932	1.524856	-0.658880
C	-1.244998	0.487312	-0.459277
C	-0.702711	-0.837099	-0.264264
H	-2.317190	0.626200	-0.422644
O	1.712134	2.355735	-1.045593
O	-0.828080	2.765718	-0.824397
O	-1.415976	-1.810673	-0.061053
H	-0.036567	3.295862	-0.996740
O	-4.194596	-2.040587	0.119204
H	-4.468923	-2.697278	-0.514450
H	-3.228124	-2.004292	0.077273
O	-4.557852	0.675194	-0.289893
H	-5.160031	1.088614	0.320997
H	-4.616264	-0.277501	-0.136026
N	0.828964	1.736249	2.037466
H	1.713845	2.146769	2.287798
H	0.116425	2.427295	2.209909
C	0.575423	0.526098	2.789614
H	0.528953	0.662015	3.872449
H	1.353355	-0.201383	2.571911
H	-0.370534	0.095899	2.468006

RC-H11

C	-0.629956	-1.278192	-0.303638
C	-1.643861	-0.348026	-0.100424
C	-2.910492	-0.777626	0.252653
C	-3.161217	-2.130295	0.403348
C	-2.150448	-3.057148	0.195714
C	-0.884407	-2.632511	-0.162791
H	-3.680543	-0.037346	0.401704
H	-4.148797	-2.465108	0.680847
H	-2.352495	-4.110666	0.311334
H	-0.082766	-3.332646	-0.337588
C	0.712126	-0.827631	-0.699060
C	0.963479	0.640769	-0.739032
C	-0.035786	1.527809	-0.588761
C	-1.376386	1.104376	-0.262566
H	0.151693	2.588270	-0.662081
O	1.578269	-1.603992	-1.048686
O	2.192569	1.031141	-0.993039
O	-2.285286	1.904353	-0.095172
H	2.831642	0.302274	-0.916462
O	-1.290816	4.551352	-0.264507
H	-1.887242	5.208918	-0.609060
H	-1.795255	3.733269	-0.189826
O	4.136997	-0.908767	-0.469294
H	4.976019	-0.986729	-0.915906
H	3.558104	-1.600834	-0.798956
N	1.946629	-0.250814	1.780458
H	2.897677	-0.445936	1.504949
H	1.669215	-0.961605	2.437579
C	1.825534	1.072162	2.357244
H	2.114741	1.811953	1.615100
H	2.430137	1.234532	3.252409
H	0.786095	1.262542	2.612203

RC-H12

C	0.376379	0.037879	-0.690278
C	-0.925666	0.653554	-0.408772
C	-2.057986	-0.145827	-0.282603
C	-1.955584	-1.625540	-0.409469
C	-0.638054	-2.203621	-0.599393
C	0.470858	-1.448743	-0.675543
O	1.371181	0.689709	-0.936707
O	-2.950108	-2.316715	-0.331153
N	1.613461	0.385796	2.504534
H	-0.572960	-3.278776	-0.638378
O	1.666191	-1.974644	-0.811636
H	1.236211	1.216430	2.080479
C	0.571953	-0.500157	2.968620
H	2.228888	-0.050002	1.835899
H	2.973895	1.781829	-1.252172
O	3.916591	1.878597	-1.097582
O	3.771961	-0.582141	0.113395
H	4.027131	0.271644	-0.267851
H	4.563785	-1.029723	0.398138
H	4.319194	2.087588	-1.935987
C	-1.023040	2.031100	-0.283534
C	-2.251852	2.608634	-0.024740
C	-3.380773	1.812058	0.099055
C	-3.286030	0.437340	-0.031666
H	-0.132296	2.630453	-0.389399
H	-2.332260	3.679280	0.079946
H	-4.338720	2.266636	0.299101
H	-4.149026	-0.203417	0.058480
H	2.388535	-1.338780	-0.628571
H	-0.003212	-0.007531	3.748898
H	1.022976	-1.382658	3.414789
H	-0.134124	-0.842054	2.204281

RC-H13

C	-1.004009	1.384361	0.728108
C	0.267947	1.184985	1.391581
C	0.838166	-0.026196	1.417061
C	0.176405	-1.222646	0.827125
C	-1.154236	-1.062072	0.243114
C	-1.737147	0.201623	0.210498
O	-1.471425	2.503245	0.579413
O	0.775264	-2.276872	0.883957
H	0.768752	2.050195	1.794049
H	-0.062188	3.586075	-0.179692
N	3.134677	-1.241490	-1.401662
H	2.734518	-2.028643	-0.920155
H	2.476205	-0.477567	-1.362158
O	0.786183	3.625051	-0.634851
H	0.885648	4.504396	-0.987641
H	1.010963	1.923666	-1.432450
O	0.957233	0.997340	-1.699962
H	0.884977	0.994147	-2.650550
C	4.418042	-0.873641	-0.852690
H	5.109011	-1.708839	-0.943738
H	4.835199	-0.053150	-1.431550
H	4.407024	-0.559829	0.196590
O	2.013641	-0.271623	1.959615
H	2.203946	-1.207957	1.807493
C	-1.824695	-2.160862	-0.267462
C	-3.086855	-1.997101	-0.808237
C	-3.670350	-0.739718	-0.840091
C	-2.996447	0.360151	-0.335822
H	-1.345094	-3.126489	-0.233836
H	-3.616542	-2.848212	-1.206566
H	-4.655331	-0.615986	-1.262984
H	-3.427928	1.348214	-0.359668

RC-P1

C	1.718669	-0.646538	-0.147889
C	2.668354	0.316583	0.184094
C	3.986718	-0.052606	0.393206
C	4.355472	-1.379460	0.270487
C	3.409831	-2.339562	-0.060489
C	2.092741	-1.975377	-0.269317
H	4.701737	0.713518	0.649275
H	5.382244	-1.668879	0.432283
H	3.703085	-3.373497	-0.155764
H	1.339071	-2.702218	-0.528521
C	0.309194	-0.261169	-0.373390
C	-0.049795	1.160422	-0.246073
C	0.863701	2.076442	0.074733
C	2.276207	1.737877	0.315012
H	0.610006	3.120933	0.173747
O	-0.527950	-1.097155	-0.653665
H	-1.083326	1.428872	-0.425108
O	3.078586	2.596345	0.606595
O	-3.185039	2.002935	-0.835642
H	-3.520152	2.488182	-1.583574
H	-3.356408	1.061266	-1.015986
O	-3.383974	-0.690361	-1.146707
H	-3.894032	-1.063664	-0.406582
H	-2.469566	-0.960103	-1.027876
N	-5.050291	-1.343265	1.047916
H	-5.611165	-2.178069	0.994379
H	-4.527956	-1.393281	1.907867
C	-5.881187	-0.150521	1.015603
H	-6.587239	-0.074665	1.843880
H	-6.442744	-0.135183	0.086153
H	-5.243940	0.728980	1.019889

RC-P2

C	-1.649146	-0.669081	0.010414
C	-2.532532	0.407637	-0.018996
C	-3.891264	0.194576	0.144903
C	-4.366431	-1.089354	0.337336
C	-3.487046	-2.162420	0.366581
C	-2.130189	-1.954275	0.203548
H	-4.553264	1.045899	0.118102
H	-5.424551	-1.257258	0.465283
H	-3.862938	-3.162504	0.517185
H	-1.426139	-2.771293	0.222901
C	-0.196440	-0.450315	-0.162489
C	0.272898	0.930040	-0.369479
C	-0.576524	1.956111	-0.395870
C	-2.028441	1.784031	-0.225038
H	-0.240173	2.970724	-0.545932
O	0.587735	-1.376978	-0.135821
H	1.336918	1.072619	-0.498694
O	-2.772609	2.738652	-0.254506
O	3.570848	1.567951	-0.706127
H	3.696523	0.584757	-0.695228
H	4.106935	1.922969	-1.409470
O	4.418966	1.072948	1.917124
H	4.158712	1.517269	1.100854
H	4.245829	1.676180	2.633146
N	3.744356	-1.078126	-0.149012
H	2.779980	-1.379137	-0.122345
H	4.028406	-0.896759	0.803987
C	4.590436	-2.078796	-0.768317
H	5.617504	-1.724264	-0.790748
H	4.579228	-3.044834	-0.260675
H	4.275099	-2.237000	-1.796201

RC-P3

C	-1.816372	0.559015	-0.230583
C	-1.309652	-0.736520	-0.192234
C	-2.080911	-1.769668	0.312949
C	-3.357327	-1.509321	0.776369
C	-3.862111	-0.217602	0.739809
C	-3.093012	0.816449	0.237650
H	-1.662620	-2.763557	0.337296
H	-3.961481	-2.312780	1.168570
H	-4.858266	-0.018637	1.103911
H	-3.460848	1.829868	0.200656
C	-1.000216	1.665852	-0.775310
C	0.318541	1.326432	-1.337127
C	0.806301	0.090045	-1.295274
C	0.055759	-1.010701	-0.674465
H	1.780604	-0.161464	-1.688304
O	-1.401409	2.807580	-0.796485
H	0.865228	2.149324	-1.771873
O	0.545241	-2.123882	-0.590768
O	0.737917	0.675186	1.684758
H	1.702663	0.531335	1.615650
H	0.521758	0.632270	2.611534
O	3.320482	-1.999207	-0.816015
H	3.802408	-2.797700	-1.009993
H	2.383798	-2.235437	-0.772655
N	3.505586	0.245109	1.264775
H	4.022481	-0.015123	2.089666
H	3.552763	-0.541934	0.628768
C	4.087136	1.426701	0.656122
H	5.126815	1.305197	0.346628
H	4.032237	2.262430	1.348502
H	3.506694	1.698945	-0.221143

RC-P4

C	1.801483	-0.562151	-0.234884
C	1.302994	0.736654	-0.197594
C	2.087590	1.768334	0.289705
C	3.368966	1.503299	0.736380
C	3.865488	0.208338	0.700989
C	3.083150	-0.824257	0.216594
H	1.675644	2.764874	0.313614
H	3.983486	2.305586	1.114617
H	4.865558	0.005681	1.052090
H	3.444381	-1.840097	0.180916
C	0.971132	-1.667465	-0.760707
C	-0.354400	-1.323770	-1.304103
C	-0.834194	-0.084192	-1.263326
C	-0.067511	1.016279	-0.661680
H	-1.812003	0.171118	-1.645394
O	1.365540	-2.811522	-0.782116
H	-0.911996	-2.146186	-1.725867
O	-0.548688	2.133118	-0.579161
O	-0.718191	-0.654049	1.717611
H	-1.683902	-0.521189	1.641107
H	-0.507901	-0.601153	2.645209
O	-3.326819	2.021042	-0.772185
H	-3.809898	2.821977	-0.952749
H	-2.389248	2.255236	-0.738699
N	-3.484479	-0.267250	1.260294
H	-4.032296	-0.058369	2.079772
H	-3.542086	0.541866	0.653606
C	-4.006441	-1.442847	0.589115
H	-5.039442	-1.343562	0.250849
H	-3.944280	-2.302542	1.250826
H	-3.388949	-1.660542	-0.278078

RC-P5

C	-1.616440	-0.763464	0.191697
C	-1.554847	0.626848	0.218060
C	-2.516432	1.377100	-0.437855
C	-3.539840	0.739697	-1.114666
C	-3.600720	-0.646234	-1.142098
C	-2.639503	-1.398313	-0.491732
H	-2.442393	2.452848	-0.407060
H	-4.292596	1.321897	-1.623286
H	-4.400970	-1.139281	-1.672138
H	-2.662371	-2.476822	-0.500923
C	-0.592442	-1.569855	0.890342
C	0.412829	-0.849257	1.690667
C	0.475862	0.479024	1.711711
C	-0.456220	1.309238	0.930120
H	1.223723	1.016914	2.273809
O	-0.581430	-2.779711	0.837529
H	1.099606	-1.471033	2.245023
O	-0.317158	2.514679	0.889483
O	1.159602	-0.099003	-1.415970
H	2.004216	-0.502983	-1.121224
H	1.015523	-0.353284	-2.322911
O	2.475913	2.121711	-0.239899
H	1.895578	1.591457	-0.798032
H	1.903106	2.757451	0.185557
N	3.604278	-0.673855	-0.259393
H	3.548904	0.246825	0.157481
H	3.604112	-1.351591	0.485723
C	4.802039	-0.796428	-1.069807
H	5.731719	-0.671678	-0.512512
H	4.778792	-0.043766	-1.852515
H	4.821980	-1.771507	-1.549015

RC-P6

C	-1.789791	-0.637505	-0.043677
C	-2.614937	0.477713	0.080209
C	-3.983613	0.316088	0.215078
C	-4.526873	-0.955362	0.226022
C	-3.705575	-2.066970	0.102652
C	-2.338801	-1.909818	-0.031444
H	-4.599309	1.196869	0.309514
H	-5.593137	-1.083080	0.330754
H	-4.134644	-3.056866	0.111576
H	-1.679673	-2.757930	-0.128934
C	-0.327832	-0.472826	-0.186032
C	0.220037	0.890471	-0.206634
C	-0.575279	1.953212	-0.083721
C	-2.034857	1.840019	0.068206
H	-0.180116	2.957571	-0.091142
O	0.399255	-1.444099	-0.281058
H	1.290425	1.003447	-0.324924
O	-2.727235	2.827317	0.176015
O	3.245380	1.882464	-0.548878
H	3.543157	2.542180	-1.168049
H	3.978816	1.238195	-0.456375
O	3.138268	-2.267192	-0.319513
H	3.042614	-3.193535	-0.119754
H	2.245986	-1.905462	-0.343617
N	5.205631	-0.083824	-0.184076
H	5.913585	-0.162375	-0.896323
H	4.617938	-0.906008	-0.254805
C	5.809584	-0.000648	1.131815
H	6.417241	0.897685	1.203831
H	6.435460	-0.856936	1.391217
H	5.024508	0.078861	1.878185

RC-P7

C	1.816276	-0.645340	0.040290
C	2.654690	0.466097	-0.001177
C	4.029166	0.298098	-0.002956
C	4.565086	-0.975932	0.037019
C	3.730595	-2.083758	0.078703
C	2.358009	-1.920277	0.079543
H	4.655172	1.176049	-0.036050
H	5.635877	-1.108622	0.036017
H	4.153902	-3.075671	0.110299
H	1.688583	-2.765349	0.111258
C	0.348336	-0.473649	0.038709
C	-0.192117	0.892376	0.010094
C	0.616038	1.951633	-0.032448
C	2.082811	1.831370	-0.043080
H	0.226069	2.957609	-0.060884
O	-0.389576	-1.441301	0.058264
H	-1.267911	1.011879	0.023926
O	2.787344	2.815175	-0.081998
O	-3.210881	1.951459	0.039964
H	-3.583983	2.645198	0.575343
H	-3.938097	1.320811	-0.146675
O	-3.131609	-2.204431	-0.213689
H	-3.035133	-3.129717	-0.418009
H	-2.239118	-1.864914	-0.086880
N	-5.158652	0.003752	-0.482308
H	-4.555797	-0.810258	-0.499303
H	-5.561357	0.099722	-1.400583
C	-6.194770	-0.156498	0.519045
H	-5.731065	-0.266976	1.495259
H	-6.843066	-1.020202	0.358278
H	-6.820458	0.732238	0.551380

RC-P8

C	1.765686	-0.631774	-0.024964
C	2.621992	0.457741	0.116550
C	3.968752	0.253259	0.364432
C	4.459397	-1.035243	0.470392
C	3.607236	-2.121159	0.329831
C	2.261916	-1.921443	0.082388
H	4.609732	1.114518	0.469664
H	5.508703	-1.196359	0.663160
H	3.995195	-3.124411	0.413604
H	1.579624	-2.749116	-0.030606
C	0.328524	-0.418595	-0.291600
C	-0.164242	0.961826	-0.401298
C	0.661328	1.999610	-0.264747
C	2.099673	1.838785	0.003166
H	0.310648	3.017328	-0.345037
O	-0.427314	-1.365690	-0.418210
H	-1.223069	1.093223	-0.597981
O	2.820716	2.803383	0.124868
O	-3.302868	1.265814	-1.017581
H	-3.408825	0.465509	-1.532187
H	-3.797251	1.065563	-0.206419
O	-3.193366	-1.679176	-1.019507
H	-3.257700	-2.505587	-1.490035
H	-2.259533	-1.565106	-0.801744
N	-4.743715	-0.009924	1.106485
H	-4.407782	-0.853225	0.662091
H	-4.419783	-0.015246	2.059615
C	-6.188590	0.077583	1.046873
H	-6.713201	-0.743517	1.540785
H	-6.501809	0.098620	0.006673
H	-6.516321	1.009075	1.500339

RC-P9

C	-0.490888	-0.682622	-0.706024
C	0.915415	-0.794666	-0.269485
C	1.766510	0.304149	-0.352555
C	1.275520	1.598781	-0.875838
C	-0.133698	1.671955	-1.287231
C	-0.956905	0.631310	-1.177241
O	-1.210298	-1.664455	-0.773423
O	1.998841	2.567667	-0.961554
N	-1.137653	0.319387	1.711936
H	-0.463811	2.629127	-1.660852
H	-1.997332	0.691348	-1.459879
H	-1.021717	-0.469486	2.326765
C	-0.408654	1.469639	2.186244
H	-2.128847	0.506340	1.630638
H	-2.986797	-1.486560	-1.030059
O	-3.917906	-1.218701	-1.080986
O	-4.104428	0.553413	1.047672
H	-4.179330	-0.069329	0.310714
H	-4.775681	1.216714	0.920222
H	-4.431281	-2.014560	-1.186300
C	1.392532	-2.006700	0.202370
C	2.710128	-2.116613	0.604254
C	3.558098	-1.019836	0.527706
C	3.088848	0.187484	0.046954
H	0.716071	-2.845741	0.246393
H	3.082021	-3.059101	0.975597
H	4.586874	-1.111588	0.839936
H	3.727113	1.053778	-0.031003
H	-0.742166	1.855274	3.153218
H	-0.501861	2.278674	1.463528
H	0.649208	1.228721	2.268940

RC-P10

C	1.753085	0.310732	-0.370874
C	0.912410	-0.793382	-0.258409
C	1.409712	-1.998153	0.211303
C	2.737304	-2.095357	0.582192
C	3.575190	-0.993309	0.475938
C	3.085644	0.206621	-0.003081
H	0.740916	-2.841814	0.277889
H	3.124952	-3.032093	0.951996
H	4.611954	-1.075273	0.763516
H	3.715570	1.076628	-0.104088
C	1.239957	1.597352	-0.893106
C	-0.180703	1.658617	-1.264550
C	-0.993452	0.613103	-1.126040
C	-0.504087	-0.695638	-0.664392
H	-2.042712	0.666670	-1.374926
O	1.955050	2.569444	-1.007415
H	-0.528589	2.611888	-1.631897
O	-1.214173	-1.685332	-0.716036
O	-3.920720	-1.282804	-1.054257
H	-4.429540	-2.087319	-1.096669
H	-2.987034	-1.539775	-0.991649
O	-4.043278	0.630501	0.944251
H	-4.147961	-0.040185	0.254174
H	-4.766135	1.243347	0.851601
N	-1.124117	0.316246	1.753743
H	-2.108851	0.526152	1.655255
H	-1.033507	-0.469387	2.376754
C	-0.372714	1.454055	2.222650
H	-0.698957	1.851608	3.187306
H	-0.450525	2.260994	1.495874
H	0.680140	1.192522	2.306532

RC-P11

C	1.706895	0.623371	0.066625
C	2.048064	-0.718829	-0.085860
C	3.376195	-1.105573	-0.028819
C	4.359766	-0.156224	0.180733
C	4.020243	1.180513	0.333013
C	2.695821	1.571790	0.274712
H	3.613845	-2.150726	-0.151025
H	5.395071	-0.456752	0.226056
H	4.791678	1.916730	0.496954
H	2.406276	2.604448	0.389219
C	0.293311	1.044369	0.000906
C	-0.727426	0.008786	-0.190415
C	-0.403242	-1.274926	-0.346275
C	0.994860	-1.737358	-0.308817
H	-1.176847	-2.013123	-0.506360
O	-0.009388	2.221642	0.097288
H	-1.760658	0.327610	-0.209692
O	1.266709	-2.908182	-0.450358
O	-4.191559	1.076141	-0.030219
H	-3.710386	1.903894	-0.174565
H	-4.806308	1.249772	0.676853
O	-2.567318	3.290472	-0.296289
H	-2.532437	3.874256	-1.048590
H	-1.663671	2.987693	-0.132122
N	-3.605471	-1.908371	-0.376127
H	-4.168796	-2.566030	-0.888973
H	-3.931332	-0.978625	-0.597245
C	-3.709165	-2.135042	1.048657
H	-3.317706	-3.118982	1.297812
H	-4.722693	-2.065676	1.454593
H	-3.097218	-1.401735	1.569831

RC-P12

C	1.709575	-0.630528	-0.090596
C	2.419622	0.552912	0.098762
C	3.800826	0.525761	0.189484
C	4.471599	-0.679549	0.091320
C	3.765388	-1.858942	-0.096902
C	2.386205	-1.836292	-0.187952
H	4.325926	1.456587	0.336225
H	5.548014	-0.702625	0.161638
H	4.293628	-2.796639	-0.172531
H	1.815033	-2.739496	-0.333995
C	0.236063	-0.606012	-0.188166
C	-0.450861	0.688937	-0.082374
C	0.236489	1.816725	0.099210
C	1.704112	1.845010	0.204457
H	-0.255889	2.774218	0.178037
O	-0.393022	-1.636296	-0.353053
H	-1.535574	0.690911	-0.162185
O	2.295221	2.888331	0.369998
O	-4.794862	-1.249882	1.465773
H	-4.250760	-1.732920	0.830708
H	-4.595843	-1.607962	2.325374
O	-3.139017	-2.277449	-0.539161
H	-3.144440	-3.148637	-0.925059
H	-2.213666	-2.006407	-0.482414
N	-3.742124	0.956737	-0.402405
H	-3.941037	0.340183	-1.174600
H	-4.168096	0.523535	0.405325
C	-4.300892	2.270891	-0.639921
H	-5.383131	2.285923	-0.793837
H	-3.834250	2.718243	-1.514875
H	-4.080375	2.916818	0.206627

RC-P13

C	-0.773579	0.897207	-0.225860
C	-1.623351	-0.147565	-0.577816
C	-2.994618	0.040800	-0.563110
C	-3.516312	1.265400	-0.188780
C	-2.670469	2.306704	0.167900
C	-1.300981	2.124455	0.148071
H	-3.629761	-0.783475	-0.847904
H	-4.585278	1.413079	-0.176718
H	-3.082556	3.260930	0.457385
H	-0.621421	2.918114	0.416222
C	0.690815	0.710080	-0.250629
C	1.218671	-0.592179	-0.671095
C	0.400625	-1.593518	-0.992915
C	-1.066402	-1.459417	-0.981816
H	0.777515	-2.558724	-1.295532
O	1.436805	1.620328	0.071481
H	2.294013	-0.710050	-0.691346
O	-1.776862	-2.371932	-1.337354
O	4.249215	1.699375	0.134144
H	4.536109	2.449374	-0.378966
H	3.282847	1.725855	0.146677
O	4.512489	-0.946710	-0.649624
H	5.164649	-1.440500	-0.161967
H	4.607063	-0.022670	-0.381220
N	-0.781321	-1.949701	1.884472
H	-1.737778	-1.903470	2.195071
H	-0.493832	-2.912934	1.939928
C	0.075556	-1.094392	2.674818
H	0.126170	-1.345588	3.737255
H	-0.268369	-0.066046	2.592128
H	1.086971	-1.129934	2.275889

RC-P14

C	-0.745007	1.017237	-0.461182
C	0.594054	1.261146	-0.167763
C	0.993852	2.521763	0.248539
C	0.060707	3.533913	0.368217
C	-1.272515	3.291416	0.067652
C	-1.675607	2.036162	-0.348613
H	2.037171	2.685055	0.468515
H	0.370156	4.515680	0.691541
H	-1.996968	4.086171	0.157242
H	-2.705008	1.823205	-0.590596
C	-1.176668	-0.324869	-0.904974
C	-0.146733	-1.371744	-1.008468
C	1.140737	-1.129935	-0.765697
C	1.598093	0.187175	-0.308823
H	1.899830	-1.892572	-0.861988
O	-2.323903	-0.538916	-1.250628
H	-0.498937	-2.347566	-1.307811
O	2.771033	0.388500	-0.047757
O	4.204416	-2.041815	-0.359486
H	5.156189	-2.060731	-0.384469
H	3.943728	-1.128106	-0.204242
O	-2.786069	-3.117497	-0.221513
H	-3.533587	-3.655518	-0.464765
H	-2.851389	-2.297382	-0.723868
N	-1.308997	-1.221962	1.655877
H	-1.730294	-2.116251	1.450626
H	-2.007758	-0.645172	2.094462
C	-0.120710	-1.333719	2.466334
H	0.614016	-1.944595	1.946766
H	-0.278184	-1.774119	3.454169
H	0.318981	-0.347802	2.607020

RC-O2

C	1.332863	-0.421414	-0.376486
C	2.293263	0.550850	-0.085222
C	3.599226	0.150925	0.160255
C	3.942292	-1.189700	0.118544
C	2.984298	-2.146527	-0.173117
C	1.679032	-1.758948	-0.421578
H	4.349047	0.894579	0.386244
H	4.960941	-1.487707	0.313168
H	3.254349	-3.190393	-0.205735
H	0.910573	-2.480877	-0.650136
C	-0.056295	-0.015235	-0.646667
C	-0.386439	1.483417	-0.603340
C	0.694249	2.406945	-0.284959
C	1.930141	1.957105	-0.049842
H	0.447439	3.456597	-0.260296
O	-0.927288	-0.795740	-0.934911
O	-1.507009	1.844975	-0.870673
H	2.721542	2.658169	0.176715
O	-2.762404	-0.679244	2.193604
H	-3.216153	-0.512047	1.330101
H	-2.777481	-1.620845	2.338403
O	-0.320686	0.519489	1.979228
H	-1.173971	0.067167	2.110476
H	-0.324786	1.261747	2.576821
N	-3.865301	-0.117783	-0.257695
H	-4.623300	0.544309	-0.211453
H	-3.072852	0.362758	-0.665021
C	-4.229760	-1.265998	-1.065520
H	-4.534713	-1.013530	-2.082622
H	-5.046103	-1.806983	-0.592526
H	-3.375542	-1.932812	-1.130656

RC-O1

C	1.301999	-0.165272	-0.489336
C	1.980826	0.811226	0.246363
C	3.293752	0.570590	0.632015
C	3.919125	-0.616192	0.292661
C	3.241161	-1.575446	-0.442510
C	1.933741	-1.346224	-0.835068
H	3.825864	1.320451	1.198684
H	4.939049	-0.790993	0.598226
H	3.732137	-2.497692	-0.711242
H	1.382336	-2.071122	-1.413877
C	-0.091962	0.066642	-0.920911
C	-0.736694	1.395831	-0.534926
C	0.057204	2.333593	0.252101
C	1.319535	2.055421	0.592796
H	-0.417683	3.266085	0.513454
O	-0.689583	-0.711290	-1.626262
O	-1.849672	1.664886	-0.929415
H	1.895478	2.777471	1.154916
O	-3.608341	-0.515536	-1.254523
H	-3.043715	0.264709	-1.333020
H	-3.071804	-1.211583	-1.628420
O	-3.890760	-0.549042	1.479687
H	-4.729292	-0.191374	1.754915
H	-3.914419	-0.596707	0.509747
N	-0.940476	-0.393252	1.424580
H	-0.342665	-0.105783	2.183219
H	-1.878778	-0.058047	1.610324
C	-0.975020	-1.833736	1.293882
H	-1.450987	-2.334651	2.136924
H	0.035783	-2.217888	1.179051
H	-1.533126	-2.090864	0.396749

RC-O3

C	1.486207	-0.300421	-0.465848
C	2.251777	0.720289	0.104180
C	3.591565	0.481397	0.375224
C	4.157312	-0.749046	0.087450
C	3.391257	-1.754444	-0.478990
C	2.054529	-1.526806	-0.755904
H	4.192417	1.263476	0.815311
H	5.199770	-0.922762	0.305288
H	3.834672	-2.712089	-0.702465
H	1.431469	-2.290600	-1.194505
C	0.064399	-0.063379	-0.763229
C	-0.518408	1.317941	-0.432583
C	0.373557	2.305151	0.162091
C	1.655083	2.011826	0.399943
H	-0.048191	3.272644	0.384409
O	-0.646084	-0.884659	-1.285341
O	-1.669637	1.548231	-0.711755
H	2.304983	2.759914	0.832599
O	-2.784552	-1.507409	1.852806
H	-3.173874	-1.307105	0.965274
H	-2.781402	-2.455323	1.948421
O	-0.411020	-0.155862	1.901578
H	-0.465357	0.451615	2.633791
H	-1.233277	-0.677558	1.928810
N	-3.717863	-0.771627	-0.619334
H	-4.012486	-1.512291	-1.235601
H	-2.854337	-0.400891	-0.995602
C	-4.725192	0.270640	-0.546819
H	-5.631309	-0.123307	-0.093487
H	-4.983400	0.702949	-1.514753
H	-4.356788	1.071416	0.086446

RC-O4

C	1.019325	-0.254180	-0.602436
C	1.827037	0.770725	-0.099359
C	3.151038	0.491311	0.215036
C	3.660881	-0.782464	0.038494
C	2.854303	-1.792191	-0.462127
C	1.536325	-1.524001	-0.787301
H	3.781515	1.278379	0.601622
H	4.689950	-0.987805	0.289446
H	3.253302	-2.784641	-0.601624
H	0.891588	-2.290266	-1.188307
C	-0.385342	0.025007	-0.958645
C	-0.917223	1.432361	-0.689545
C	0.013715	2.423294	-0.166518
C	1.285296	2.103051	0.093429
H	-0.372544	3.418726	-0.013737
O	-1.097200	-0.779926	-1.509589
O	-2.067385	1.699074	-0.963621
H	1.962159	2.856323	0.472334
O	-2.360133	-2.540662	0.463570
H	-3.060897	-1.891706	0.323104
H	-1.895651	-2.549750	-0.371994
O	-3.871475	-0.223443	0.012615
H	-4.766507	-0.076254	-0.279194
H	-3.303706	0.312153	-0.557337
N	-1.049124	0.001166	1.527471
H	-1.863391	0.553617	1.749390
H	-1.377797	-0.944157	1.359060
C	-0.060249	0.049916	2.578131
H	-0.444250	-0.233368	3.560432
H	0.350886	1.055281	2.653380
H	0.758116	-0.622010	2.332368

RC-O5

C	1.020841	-0.008524	0.534849
C	1.944969	-0.683704	-0.268165
C	3.147786	-0.060836	-0.570293
C	3.426048	1.204828	-0.083565
C	2.508405	1.863277	0.718636
C	1.305538	1.252819	1.026616
H	3.867941	-0.571588	-1.191944
H	4.364728	1.677184	-0.328613
H	2.731231	2.846530	1.102165
H	0.575805	1.739218	1.655362
C	-0.263983	-0.647682	0.851684
C	-0.523719	-2.055140	0.299958
C	0.518527	-2.668921	-0.509331
C	1.655381	-2.017559	-0.765932
H	0.321020	-3.658104	-0.890057
O	-1.108040	-0.126219	1.542955
O	-1.565484	-2.599818	0.574313
H	2.416360	-2.485305	-1.374472
O	-1.119924	-0.237316	-1.598176
H	-2.006048	-0.591083	-1.493067
H	-1.240971	0.691726	-1.328382
O	-3.571992	-0.442770	0.047883
H	-4.120835	-1.222679	0.059411
H	-2.907311	-0.598846	0.727850
N	-1.972033	2.174386	-0.388912
H	-2.946526	1.951295	-0.525864
H	-1.769541	1.934925	0.569972
C	-1.696655	3.570102	-0.658903
H	-2.259478	4.270933	-0.038361
H	-1.920372	3.787974	-1.699585
H	-0.637082	3.764148	-0.511153

RC-O6

C	1.168686	0.187589	0.527711
C	2.117486	-0.371539	-0.333327
C	3.221255	0.387221	-0.698115
C	3.378938	1.675394	-0.216096
C	2.437717	2.219749	0.642148
C	1.333844	1.472075	1.013463
H	3.960432	-0.035995	-1.362057
H	4.241724	2.254014	-0.507750
H	2.565874	3.221323	1.021620
H	0.589232	1.866801	1.687499
C	-0.011972	-0.601282	0.923948
C	-0.139281	-2.027078	0.367933
C	0.913622	-2.506090	-0.519007
C	1.952652	-1.727148	-0.831464
H	0.809256	-3.509628	-0.899706
O	-0.860464	-0.184615	1.669381
O	-1.083940	-2.701062	0.694939
H	2.726041	-2.101732	-1.487618
O	-1.174944	-0.232110	-1.547258
H	-1.540998	0.608836	-1.183552
H	-0.883090	-0.062405	-2.438300
O	-3.484952	-1.066355	0.030286
H	-2.876611	-1.145287	-0.708099
H	-3.030696	-1.513376	0.745574
N	-2.455949	1.744048	-0.151984
H	-3.047326	0.986054	0.172741
H	-1.911019	2.039418	0.642428
C	-3.243963	2.836961	-0.685588
H	-3.929565	3.285085	0.035834
H	-3.833568	2.477404	-1.524426
H	-2.587542	3.619177	-1.058723

RC-O7

C	-1.872522	-0.543071	0.038847
C	-0.484046	-0.711862	0.065682
C	0.048542	-1.948963	0.403859
C	-0.799003	-3.001093	0.712244
C	-2.174041	-2.830633	0.685798
C	-2.710870	-1.599800	0.348675
H	1.124923	-2.067360	0.418361
H	-0.382061	-3.961437	0.974484
H	-2.826542	-3.655334	0.926860
H	-3.777240	-1.437536	0.318691
C	-2.446241	0.767672	-0.318408
C	-1.467964	1.912222	-0.648923
C	-0.041574	1.613149	-0.600946
C	0.400265	0.393615	-0.264805
H	0.637872	2.410667	-0.863288
O	-3.629886	0.977140	-0.356180
O	-1.907073	3.000425	-0.922346
H	1.463195	0.197519	-0.234074
O	1.921697	2.739246	1.946201
H	1.942175	2.728410	2.899678
H	1.028183	2.523650	1.682737
O	3.591399	1.463902	0.087047
H	3.132874	1.944835	0.786478
H	4.164010	2.091680	-0.344359
N	3.446981	-1.604694	-0.095878
H	3.717222	-0.656483	0.124750
H	4.102560	-2.221690	0.354766
C	3.454396	-1.805383	-1.529688
H	4.422465	-1.644982	-2.011509
H	2.742729	-1.123782	-1.990522
H	3.128006	-2.816116	-1.763697

Cartesian coordinates of products

P-H1-1

C	0.474107	-0.534377	-0.200003
C	1.167174	0.649420	0.012524
C	2.548638	0.630306	0.153055
C	3.238621	-0.561921	0.079198
C	2.548454	-1.745834	-0.141006
C	1.174231	-1.729573	-0.282600
H	3.051235	1.570371	0.319070
H	4.311709	-0.574622	0.190508
H	3.083519	-2.680886	-0.204204
H	0.639796	-2.650146	-0.468246
C	-1.021799	-0.548546	-0.396409
C	-1.662624	0.805155	-0.163779
C	-0.984411	1.945035	0.007144
C	0.459609	1.956687	0.100194
H	-1.500926	2.884603	0.116437
O	-2.984490	0.764568	-0.194651
O	1.088385	2.983940	0.261445
H	-3.230872	-0.172655	-0.192842
O	-1.334997	-0.968667	-1.704773
N	-1.754776	-1.486498	0.416220
H	-0.791831	-0.485850	-2.326898
H	-1.606912	-2.414483	0.052988
C	-1.511813	-1.399586	1.839395
H	-2.139890	-2.124207	2.346925
H	-1.794375	-0.410617	2.193709
H	-0.470331	-1.575349	2.116566

P-H1-2

C	0.478594	-0.574737	-0.246011
C	1.055910	0.679944	-0.105851
C	2.437163	0.808975	-0.076003
C	3.240703	-0.307613	-0.188653
C	2.663327	-1.560693	-0.331393
C	1.287079	-1.693365	-0.354399
H	2.850180	1.799702	0.032463
H	4.314694	-0.206445	-0.169569
H	3.287203	-2.436306	-0.424474
H	0.842628	-2.671289	-0.458432
C	-1.014536	-0.733258	-0.186888
C	-1.742206	0.558336	-0.471404
C	-1.199039	1.763807	-0.285475
C	0.220402	1.908623	-0.023531
H	-1.787414	2.661426	-0.382789
O	-3.030949	0.397396	-0.770950
O	0.728944	2.988999	0.199658
H	-3.127282	-0.491531	-1.132037
O	-1.513178	-1.652079	-1.127717
N	-1.402140	-1.247302	1.115941
H	-1.478095	-2.512113	-0.705382
H	-2.408587	-1.187522	1.184151
C	-0.799032	-0.626406	2.278505
H	-1.291321	-1.017041	3.163154
H	-0.888302	0.463462	2.286118
H	0.252558	-0.887421	2.333895

P-H1-3

C	0.583399	-0.602850	-0.166956
C	1.258521	0.592731	0.045543
C	2.640240	0.596745	0.164131
C	3.348392	-0.584836	0.064969
C	2.674273	-1.776012	-0.154931
C	1.294673	-1.785733	-0.262357
H	3.131443	1.543843	0.324537
H	4.423846	-0.580162	0.151074
H	3.224169	-2.700392	-0.242406
H	0.773457	-2.715368	-0.430070
C	-0.921973	-0.619911	-0.163656
C	-1.491899	0.724797	-0.572797
C	-0.856213	1.877670	-0.342223
C	0.529553	1.890812	0.083418
H	-1.335056	2.824064	-0.532355
O	-2.725380	0.683566	-1.060381
O	1.107188	2.915296	0.387516
H	-2.896773	-0.228970	-1.321128
O	-1.476888	-1.542841	-1.071189
N	-1.337260	-1.019004	1.163376
H	-1.544222	-2.373331	-0.597723
H	-0.668636	-0.700920	1.844553
C	-2.694412	-0.715012	1.567232
H	-2.861323	-1.144448	2.549903
H	-3.396996	-1.183260	0.882651
H	-2.915786	0.353401	1.605534

P-H1-4

C	-0.412107	-0.485472	0.210355
C	-1.204878	0.622721	-0.068499
C	-2.584921	0.495696	-0.121436
C	-3.181698	-0.727110	0.114040
C	-2.396029	-1.827450	0.419166
C	-1.018146	-1.707813	0.466161
H	-3.164325	1.380452	-0.334960
H	-4.255719	-0.822074	0.075536
H	-2.856890	-2.781918	0.622418
H	-0.406549	-2.563634	0.708391
C	1.092501	-0.380324	0.182612
C	1.577165	1.049942	0.273847
C	0.807549	2.116677	0.035061
C	-0.609635	1.976734	-0.231144
H	1.223170	3.111008	0.037205
O	2.871085	1.159102	0.536123
O	-1.306015	2.925076	-0.534253
H	3.233793	0.271007	0.624215
O	1.671102	-1.124884	1.230139
N	1.729018	-0.896346	-1.006978
H	1.186273	-0.955826	2.037878
H	1.553308	-0.275984	-1.780428
C	1.466979	-2.273622	-1.356383
H	2.131840	-2.549572	-2.169312
H	0.437970	-2.468877	-1.665605
H	1.703944	-2.904382	-0.505244

P-H1-5

C	0.500454	-0.564995	-0.217245
C	1.092449	0.682017	-0.074723
C	2.475203	0.785563	-0.011942
C	3.259039	-0.347951	-0.092083
C	2.663897	-1.594742	-0.225734
C	1.286737	-1.704709	-0.277414
H	2.904959	1.768715	0.100252
H	4.333939	-0.265266	-0.046832
H	3.275504	-2.482234	-0.280257
H	0.804350	-2.667367	-0.352647
C	-0.992766	-0.724016	-0.231123
C	-1.714246	0.593455	-0.416911
C	-1.154972	1.791002	-0.227884
C	0.272255	1.921521	-0.000993
H	-1.737329	2.695830	-0.293044
O	-3.014268	0.460811	-0.686683
O	0.796908	2.998467	0.198664
H	-3.151016	-0.424789	-1.039350
O	-1.434943	-1.583505	-1.263033
N	-1.417812	-1.394209	0.971645
H	-0.976114	-1.360813	-2.073086
H	-2.396804	-1.623364	0.890357
C	-1.143702	-0.710299	2.215412
H	-1.524209	-1.318602	3.029471
H	-1.586948	0.286423	2.288086
H	-0.069310	-0.616338	2.347785

P-H1-6

C	0.418894	-0.486847	-0.206150
C	1.181853	0.639774	0.077055
C	2.564869	0.551100	0.100555
C	3.190969	-0.650530	-0.169510
C	2.432024	-1.768268	-0.476159
C	1.049837	-1.687561	-0.491304
H	3.124022	1.447054	0.321167
H	4.267838	-0.715071	-0.153757
H	2.915511	-2.706457	-0.701188
H	0.456005	-2.559865	-0.720917
C	-1.082555	-0.407455	-0.149861
C	-1.588379	1.007541	-0.313916
C	-0.856925	2.092541	-0.062456
C	0.551086	1.974588	0.267324
H	-1.284931	3.080207	-0.110315
O	-2.882016	1.070301	-0.632919
O	1.217040	2.929957	0.610277
H	-3.122764	0.220602	-1.020300
O	-1.680029	-1.192622	-1.184937
N	-1.575636	-0.849698	1.112536
H	-1.167716	-1.107377	-1.990091
H	-2.542917	-0.589625	1.214627
C	-1.355446	-2.232861	1.469611
H	-1.934837	-2.446387	2.362019
H	-0.309407	-2.393510	1.713830
H	-1.648672	-2.934907	0.686675

P-H1-7

C	-0.555483	-0.587548	0.146421
C	-1.295341	0.565979	-0.075247
C	-2.675183	0.490400	-0.177802
C	-3.316774	-0.727660	-0.055250
C	-2.577783	-1.877050	0.174453
C	-1.197815	-1.808821	0.269109
H	-3.220200	1.405818	-0.348275
H	-4.391539	-0.782652	-0.131985
H	-3.075341	-2.828949	0.279173
H	-0.615982	-2.702337	0.443308
C	0.947923	-0.533563	0.142488
C	1.465767	0.854623	0.460506
C	0.756996	1.965755	0.251516
C	-0.637253	1.899733	-0.141531
H	1.187387	2.939648	0.417363
O	2.714038	0.890293	0.921652
O	-1.276933	2.889343	-0.434450
H	2.970720	-0.012043	1.140688
O	1.510126	-1.424830	1.108321
N	1.386366	-0.915822	-1.157980
H	1.035629	-1.338485	1.936188
H	0.927398	-1.773157	-1.418340
C	2.809857	-0.972686	-1.407762
H	2.962465	-1.404845	-2.391322
H	3.360486	-1.575551	-0.681039
H	3.227103	0.029885	-1.425491

P-H1-8

C	0.488361	-0.523685	-0.190332
C	1.158466	0.677431	-0.008339
C	2.542225	0.695034	0.105331
C	3.259194	-0.481641	0.040415
C	2.589998	-1.685571	-0.127261
C	1.212443	-1.705535	-0.240094
H	3.025413	1.648910	0.248902
H	4.334420	-0.466854	0.128355
H	3.143975	-2.611117	-0.164477
H	0.683136	-2.641481	-0.344961
C	-1.005961	-0.587927	-0.408106
C	-1.675997	0.745528	-0.167613
C	-1.031360	1.891140	0.061155
C	0.418040	1.956340	0.110963
H	-1.559680	2.821420	0.212789
O	-3.003954	0.618626	-0.211644
O	1.001673	3.009362	0.269725
H	-3.428337	1.470368	-0.113660
O	-1.299889	-0.874975	-1.749020
N	-1.578442	-1.640093	0.391505
H	-0.974235	-1.758954	-1.924470
H	-2.551040	-1.708344	0.130125
C	-1.451371	-1.473834	1.823448
H	-1.934366	-2.311099	2.317134
H	-1.896156	-0.547315	2.199031
H	-0.400900	-1.482678	2.100808

P-H1-9

C	0.554390	-0.605624	-0.203229
C	1.096986	0.665327	-0.063694
C	2.471108	0.824972	0.051377
C	3.302835	-0.275617	0.015281
C	2.761770	-1.542755	-0.149665
C	1.392983	-1.708477	-0.254832
H	2.856751	1.827392	0.153874
H	4.371182	-0.150465	0.098451
H	3.410315	-2.403693	-0.204709
H	0.969804	-2.690325	-0.404074
C	-0.937206	-0.796053	-0.161760
C	-1.675719	0.448997	-0.590767
C	-1.150644	1.673529	-0.513042
C	0.234928	1.874506	-0.129688
H	-1.737880	2.544885	-0.752507
O	-2.936312	0.244612	-0.954778
O	0.697268	2.980811	0.065023
H	-3.024908	-0.685912	-1.182722
O	-1.333188	-1.851558	-1.006627
N	-1.375703	-1.176735	1.178002
H	-1.805861	-2.465987	-0.441533
H	-0.678536	-1.811818	1.540293
C	-1.583699	-0.118698	2.147145
H	-1.782215	-0.581760	3.108404
H	-2.451006	0.472307	1.872112
H	-0.726272	0.550952	2.254698

P-H1-10

C	0.550133	-0.588688	-0.145693
C	1.310607	0.554929	0.058047
C	2.691106	0.454806	0.156532
C	3.306780	-0.776430	0.048893
C	2.543560	-1.918171	-0.148672
C	1.166236	-1.826848	-0.233515
H	3.254043	1.361657	0.313583
H	4.380883	-0.850686	0.120057
H	3.022976	-2.881814	-0.227145
H	0.554458	-2.707139	-0.357948
C	-0.951168	-0.525573	-0.171307
C	-1.453459	0.885056	-0.422526
C	-0.732939	1.985730	-0.181693
C	0.676645	1.899863	0.140343
H	-1.166170	2.967063	-0.286295
O	-2.716275	0.956956	-0.835437
O	1.342358	2.879351	0.411412
H	-2.990101	0.071914	-1.098180
O	-1.514689	-1.350659	-1.173365
N	-1.423744	-1.070263	1.072780
H	-1.042911	-1.208404	-1.994143
H	-0.878430	-0.701183	1.832932
C	-2.841807	-1.027570	1.348048
H	-3.025127	-1.588508	2.259397
H	-3.374676	-1.535523	0.548141
H	-3.254057	-0.023355	1.468518

P-H1-11

C	-0.439306	-0.462683	0.258225
C	-1.135716	0.698667	-0.057686
C	-2.522570	0.691745	-0.104684
C	-3.219943	-0.466054	0.175161
C	-2.527648	-1.617331	0.518635
C	-1.144587	-1.617420	0.558269
H	-3.026076	1.614859	-0.346258
H	-4.298384	-0.470658	0.143582
H	-3.067961	-2.519618	0.761415
H	-0.602067	-2.506217	0.838869
C	1.066997	-0.497919	0.185184
C	1.661612	0.883769	0.328649
C	0.995623	2.007883	0.055457
C	-0.425313	1.985766	-0.254626
H	1.472554	2.977029	0.072158
O	2.949234	0.814478	0.666648
O	-1.014070	2.988563	-0.604623
H	3.336948	1.687318	0.721493
O	1.521485	-1.336720	1.196702
N	1.581043	-0.984566	-1.086118
H	2.477526	-1.364913	1.121779
H	1.441538	-0.291284	-1.803685
C	1.110243	-2.282888	-1.513617
H	1.699375	-2.596110	-2.370547
H	0.052591	-2.310027	-1.784365
H	1.277104	-3.000199	-0.715239

P-H1-12

C	-0.396090	-0.513097	0.151816
C	-1.285592	0.530230	-0.078269
C	-2.648527	0.279204	-0.163345
C	-3.131888	-1.002215	-0.001593
C	-2.250793	-2.036703	0.276192
C	-0.892811	-1.792726	0.359192
H	-3.304765	1.117187	-0.339331
H	-4.191455	-1.194865	-0.066666
H	-2.624396	-3.035716	0.441040
H	-0.215669	-2.590099	0.619012
C	1.088631	-0.271388	0.211988
C	1.455896	1.192553	0.162261
C	0.594060	2.195181	0.014932
C	-0.826204	1.940520	-0.157935
H	0.932041	3.217211	-0.035572
O	2.778232	1.385517	0.263182
O	-1.611973	2.842628	-0.363702
H	3.186025	0.609635	-0.150938
O	1.531902	-0.835135	1.412049
N	1.880928	-0.836184	-0.880758
H	2.414922	-0.512071	1.598481
H	1.597585	-0.403375	-1.748001
C	1.903334	-2.277501	-1.022346
H	2.708888	-2.545489	-1.699698
H	0.972159	-2.694473	-1.407393
H	2.112786	-2.723081	-0.055229

P-H1-13

C	0.502153	-0.534889	-0.189715
C	1.155369	0.674934	0.000853
C	2.538580	0.706333	0.128427
C	3.265652	-0.463738	0.063695
C	2.611624	-1.673962	-0.127253
C	1.236324	-1.709620	-0.254089
H	3.011951	1.663823	0.280122
H	4.339762	-0.438979	0.163712
H	3.178300	-2.591281	-0.175322
H	0.706784	-2.638718	-0.397164
C	-0.990696	-0.632193	-0.388479
C	-1.676193	0.708716	-0.213006
C	-1.046386	1.870084	-0.011683
C	0.400044	1.947732	0.092276
H	-1.585583	2.801016	0.092955
O	-3.001764	0.572712	-0.284254
O	0.968788	3.007996	0.258023
H	-3.434510	1.421137	-0.193473
O	-1.288941	-1.100316	-1.681047
N	-1.545794	-1.632219	0.476854
H	-0.811779	-0.576900	-2.323380
H	-2.489681	-1.808588	0.167411
C	-1.506902	-1.312261	1.884203
H	-1.930518	-2.141045	2.442351
H	-2.052896	-0.401581	2.151241
H	-0.473352	-1.193314	2.200423

P-H1-14

C	0.433861	-0.476885	-0.202775
C	1.178658	0.660918	0.081206
C	2.564229	0.594650	0.128272
C	3.211692	-0.597430	-0.122506
C	2.470989	-1.724316	-0.445191
C	1.090002	-1.663836	-0.488147
H	3.106002	1.501318	0.348018
H	4.288902	-0.647599	-0.087639
H	2.971317	-2.653606	-0.670980
H	0.512418	-2.532547	-0.761423
C	-1.072719	-0.445088	-0.188035
C	-1.603684	0.962796	-0.267153
C	-0.889957	2.063629	-0.048340
C	0.533185	1.985585	0.239324
H	-1.334060	3.048108	-0.049484
O	-2.925419	0.933577	-0.507473
O	1.171230	2.971086	0.548063
H	-3.291863	1.817302	-0.521645
O	-1.499823	-1.174295	-1.316511
N	-1.589126	-0.950574	1.056181
H	-2.446340	-1.056286	-1.406094
H	-2.577846	-0.761650	1.102404
C	-1.309702	-2.331289	1.379716
H	-1.925157	-2.611500	2.228856
H	-0.271298	-2.444144	1.676384
H	-1.515415	-3.020713	0.557470

P-H1-15

C	-0.568781	-0.595635	0.168574
C	-1.275578	0.575958	-0.066935
C	-2.655865	0.540989	-0.180867
C	-3.334479	-0.656477	-0.055653
C	-2.630654	-1.822928	0.194495
C	-1.250138	-1.792454	0.302489
H	-3.171772	1.471420	-0.360422
H	-4.409686	-0.681487	-0.140685
H	-3.155955	-2.758288	0.311766
H	-0.712843	-2.705661	0.512805
C	0.937143	-0.566385	0.148720
C	1.476199	0.795623	0.542967
C	0.799495	1.923820	0.321895
C	-0.580301	1.891368	-0.123505
H	1.244454	2.885629	0.515980
O	2.711602	0.791871	1.032724
O	-1.183445	2.895048	-0.445244
H	2.914365	-0.113682	1.293032
O	1.512972	-1.450957	1.105384
N	1.335393	-0.854455	-1.190376
H	1.537896	-2.332588	0.738059
H	0.801226	-1.607698	-1.587235
C	2.739417	-0.871555	-1.520085
H	2.845723	-1.193430	-2.550667
H	3.339449	-1.535637	-0.890923
H	3.151611	0.130956	-1.444555

P-H1-16

C	-0.427517	-0.482653	0.241100
C	-1.157450	0.658913	-0.065863
C	-2.542701	0.613371	-0.090647
C	-3.206206	-0.562282	0.201365
C	-2.480881	-1.694426	0.535120
C	-1.097423	-1.653142	0.553825
H	-3.073078	1.522143	-0.329109
H	-4.284455	-0.595064	0.185389
H	-2.991804	-2.611489	0.785151
H	-0.545072	-2.541195	0.823968
C	1.076527	-0.441221	0.162522
C	1.617647	0.956034	0.364441
C	0.917441	2.054856	0.088566
C	-0.485068	1.969957	-0.273783
H	1.369153	3.031489	0.140610
O	2.905222	0.990187	0.705620
O	-1.114446	2.936678	-0.652401
H	3.112852	0.142868	1.116107
O	1.683062	-1.201808	1.201885
N	1.509731	-0.838674	-1.145922
H	1.684733	-2.126256	0.960357
H	2.482198	-0.609334	-1.273742
C	1.205219	-2.176126	-1.588474
H	1.682663	-2.335010	-2.549735
H	0.134794	-2.290999	-1.726800
H	1.551663	-2.976588	-0.920609

P-H1-17

C	0.425252	-0.478053	-0.174073
C	1.189520	0.652759	0.088659
C	2.573707	0.567032	0.138433
C	3.205382	-0.638746	-0.086468
C	2.449230	-1.761218	-0.386600
C	1.069332	-1.679589	-0.434921
H	3.126921	1.470733	0.341501
H	4.281668	-0.703320	-0.047687
H	2.935321	-2.703520	-0.588079
H	0.482269	-2.549665	-0.684528
C	-1.086149	-0.430129	-0.197221
C	-1.603199	0.990328	-0.239898
C	-0.858726	2.079092	-0.034794
C	0.564104	1.990197	0.225715
H	-1.293315	3.067936	-0.014796
O	-2.924835	1.005724	-0.428964
O	1.225467	2.969908	0.505096
H	-3.260843	1.899205	-0.362123
O	-1.573090	-1.150867	-1.312436
N	-1.660876	-0.973496	0.993990
H	-1.101475	-0.885915	-2.101886
H	-2.655241	-0.814683	0.947178
C	-1.386539	-2.358948	1.303337
H	-2.044229	-2.654979	2.114644
H	-0.365445	-2.472483	1.654777
H	-1.551324	-3.033297	0.460495

P-H1-18

C	0.539121	-0.571069	-0.144088
C	1.327174	0.547698	0.084067
C	2.705091	0.420298	0.189686
C	3.299348	-0.819070	0.065879
C	2.514255	-1.936295	-0.177765
C	1.140546	-1.812587	-0.282835
H	3.283477	1.314267	0.363996
H	4.370655	-0.916941	0.148085
H	2.974498	-2.905936	-0.291061
H	0.524704	-2.675044	-0.490796
C	-0.971719	-0.501291	-0.177641
C	-1.455217	0.922788	-0.351508
C	-0.689751	2.000303	-0.154219
C	0.723493	1.898750	0.156336
H	-1.094528	2.999617	-0.226116
O	-2.745075	0.976997	-0.690747
O	1.394378	2.878264	0.412485
H	-3.030469	1.888819	-0.752534
O	-1.480898	-1.309068	-1.218240
N	-1.443164	-0.999113	1.076110
H	-1.226167	-0.952087	-2.068490
H	-0.917059	-1.823226	1.312746
C	-2.868041	-1.225382	1.223375
H	-3.015742	-1.836965	2.108020
H	-3.312682	-1.726789	0.364655
H	-3.387592	-0.286332	1.383019

P-H1-19

C	0.547490	-0.575944	-0.143270
C	1.330178	0.551228	0.063361
C	2.710455	0.431078	0.166059
C	3.306057	-0.808455	0.061642
C	2.522149	-1.935868	-0.145066
C	1.148408	-1.821200	-0.241139
H	3.287082	1.329069	0.324394
H	4.378312	-0.901439	0.138637
H	2.985717	-2.907005	-0.228104
H	0.521457	-2.685639	-0.393142
C	-0.962314	-0.522915	-0.201717
C	-1.456250	0.904253	-0.347066
C	-0.705637	1.988071	-0.116341
C	0.718356	1.898183	0.147291
H	-1.125401	2.983526	-0.150521
O	-2.749302	0.954273	-0.677589
O	1.386033	2.883663	0.390131
H	-3.046922	1.863748	-0.712414
O	-1.463477	-1.300142	-1.255969
N	-1.447791	-1.156275	0.991400
H	-1.320988	-0.847628	-2.086089
H	-0.916822	-0.860259	1.791667
C	-2.871499	-1.192209	1.231914
H	-3.067766	-1.934526	2.000626
H	-3.368981	-1.506295	0.320976
H	-3.301530	-0.239320	1.547581

P-H1-20

C	0.504967	-0.531472	-0.232863
C	1.090891	0.709709	-0.029941
C	2.471072	0.824505	0.082368
C	3.269705	-0.295528	-0.010246
C	2.688146	-1.538828	-0.220192
C	1.315724	-1.654891	-0.326518
H	2.885168	1.808561	0.237910
H	4.341497	-0.206659	0.075462
H	3.307902	-2.418774	-0.300788
H	0.862518	-2.621423	-0.493889
C	-0.998672	-0.728747	-0.301780
C	-1.741401	0.590336	-0.338318
C	-1.162736	1.786256	-0.173758
C	0.263782	1.938566	0.033417
H	-1.742464	2.698326	-0.185754
O	-3.042103	0.410809	-0.531346
O	0.768359	3.026304	0.229384
H	-3.494141	1.254014	-0.551090
O	-1.326386	-1.489383	-1.432747
N	-1.520916	-1.497166	0.796323
H	-0.829649	-1.162414	-2.181504
H	-1.222968	-2.451777	0.673044
C	-1.226095	-0.999939	2.117186
H	-1.654402	-1.680755	2.845705
H	-1.700295	-0.031583	2.259680
H	-0.158028	-0.888990	2.328516

P-H1-21

C	0.431009	-0.464087	-0.236042
C	1.158732	0.683258	0.062321
C	2.544293	0.642927	0.111584
C	3.214649	-0.536657	-0.145067
C	2.495143	-1.677631	-0.463893
C	1.112108	-1.642590	-0.507562
H	3.068953	1.557839	0.339296
H	4.292539	-0.566953	-0.110370
H	3.012426	-2.599886	-0.680318
H	0.551696	-2.530606	-0.756992
C	-1.084899	-0.471014	-0.183524
C	-1.650599	0.928800	-0.305305
C	-0.943950	2.033423	-0.034593
C	0.477701	1.987569	0.250747
H	-1.401404	3.012422	-0.035023
O	-2.938197	0.917636	-0.624735
O	1.096325	2.980463	0.578722
H	-3.284660	1.809731	-0.634499
O	-1.608266	-1.308165	-1.170462
N	-1.611556	-0.971621	1.065863
H	-1.190617	-1.105249	-2.006006
H	-1.386581	-0.328749	1.807011
C	-1.276432	-2.330756	1.419199
H	-1.864531	-2.607901	2.289150
H	-0.219771	-2.491899	1.648224
H	-1.562585	-2.986316	0.603091

P-H2-2

C	-1.278045	0.535039	-0.041603
C	-0.931225	-0.823866	-0.005628
C	-1.914436	-1.801690	-0.012152
C	-3.246689	-1.448547	-0.091215
C	-3.592539	-0.104777	-0.132214
C	-2.623588	0.880444	-0.098831
H	-1.606319	-2.834518	0.042821
H	-4.011386	-2.208661	-0.115133
H	-4.632796	0.178804	-0.184888
H	-2.894593	1.923463	-0.110919
C	-0.249613	1.553304	0.033205
C	1.040133	1.226425	-0.021237
C	1.506855	-0.170590	-0.270281
C	0.478947	-1.211491	0.128098
O	-0.675754	2.832945	0.156492
O	2.000927	2.166909	0.035531
O	0.837544	-2.299907	0.515181
H	2.820445	1.676554	0.205328
H	1.603751	-0.282060	-1.358601
H	0.092745	3.403438	0.197443
N	2.818449	-0.357532	0.299707
H	2.714404	-0.703722	1.242430
C	3.670307	-1.265596	-0.446024
H	4.624328	-1.356230	0.064520
H	3.862377	-0.847333	-1.431484
H	3.235524	-2.258524	-0.559806

P-H2-1

C	-1.121694	0.634517	-0.016825
C	-0.982553	-0.753588	-0.160632
C	-2.093159	-1.581975	-0.088575
C	-3.350759	-1.046906	0.102980
C	-3.490907	0.327172	0.242016
C	-2.391128	1.162801	0.188985
H	-1.940377	-2.645456	-0.189496
H	-4.215821	-1.689523	0.146205
H	-4.470778	0.752811	0.397011
H	-2.500029	2.228288	0.308236
C	0.042795	1.496976	-0.051188
C	1.252973	1.009292	-0.315201
C	1.502662	-0.415241	-0.666794
C	0.348240	-1.347909	-0.333039
O	-0.175058	2.810760	0.191515
O	2.327190	1.825354	-0.355466
O	0.558788	-2.537547	-0.260898
H	3.100712	1.245460	-0.372505
H	1.581202	-0.470517	-1.759665
H	0.664306	3.269951	0.141069
N	2.787261	-0.808192	-0.136205
H	3.096258	-1.647781	-0.597615
C	2.793709	-0.998379	1.303425
H	3.803511	-1.234015	1.624535
H	2.123932	-1.791665	1.636459
H	2.497816	-0.069310	1.787082

P-H2-3

C	-1.115664	0.624025	-0.017601
C	-0.987375	-0.766740	-0.130472
C	-2.101866	-1.586908	-0.048998
C	-3.359295	-1.041643	0.119502
C	-3.493736	0.336014	0.213680
C	-2.387642	1.163331	0.149732
H	-1.953011	-2.652879	-0.127332
H	-4.228282	-1.678135	0.170744
H	-4.473492	0.772532	0.335335
H	-2.512204	2.233517	0.205053
C	0.064766	1.458884	-0.050174
C	1.282678	0.979912	-0.323354
C	1.518273	-0.451707	-0.668101
C	0.344742	-1.361174	-0.300077
O	-0.050378	2.818666	0.112245
O	2.356204	1.771448	-0.387769
O	0.542308	-2.550995	-0.206944
H	2.057270	2.671523	-0.230617
H	1.549352	-0.496820	-1.764568
H	-0.447309	3.015520	0.960303
N	2.781384	-0.932709	-0.184869
H	2.882977	-1.883817	-0.501866
C	2.902345	-0.884255	1.255525
H	3.850950	-1.326259	1.544084
H	2.103148	-1.411667	1.786070
H	2.912496	0.154064	1.578654

P-H2-4

C	-1.227087	0.592761	-0.003402
C	-1.045829	-0.795309	-0.067365
C	-2.138242	-1.649306	-0.083035
C	-3.421917	-1.141976	-0.062417
C	-3.606644	0.231406	0.009564
C	-2.525455	1.091532	0.046522
H	-1.950578	-2.711585	-0.109323
H	-4.271561	-1.805400	-0.089103
H	-4.606288	0.637043	0.047159
H	-2.688307	2.153573	0.142567
C	-0.076049	1.464482	0.020850
C	1.175056	1.001700	-0.048078
C	1.492947	-0.439095	-0.263215
C	0.307529	-1.359354	-0.018441
O	-0.237434	2.821368	0.178733
O	2.230531	1.820070	-0.021311
O	0.511061	-2.534971	0.182525
H	1.899186	2.712444	0.113942
H	1.656238	-0.537170	-1.355290
H	-0.745405	3.178052	-0.549590
N	2.630555	-0.905864	0.473643
H	2.476139	-1.885346	0.659618
C	3.904219	-0.710349	-0.177601
H	4.676540	-1.199549	0.408552
H	4.141973	0.346509	-0.228062
H	3.933733	-1.118212	-1.195848

P-H2-5

C	-1.090237	0.633793	-0.008151
C	-0.985624	-0.751409	-0.191460
C	-2.109092	-1.560160	-0.114289
C	-3.352195	-1.008844	0.124253
C	-3.459825	0.360910	0.316223
C	-2.344219	1.175599	0.258285
H	-1.976731	-2.623251	-0.244081
H	-4.228167	-1.635964	0.171855
H	-4.424201	0.799909	0.522444
H	-2.443189	2.233022	0.447508
C	0.092265	1.462144	-0.090126
C	1.309555	0.968920	-0.340223
C	1.547906	-0.468601	-0.649071
C	0.335947	-1.362817	-0.381210
O	0.003133	2.813464	0.147487
O	2.389312	1.751961	-0.402094
O	0.505061	-2.560651	-0.354338
H	2.102401	2.649550	-0.211444
H	1.674879	-0.518693	-1.737765
H	-0.593790	3.219054	-0.480874
N	2.758595	-0.968422	-0.058517
H	2.871980	-1.921776	-0.365069
C	2.755636	-0.914672	1.386529
H	3.671705	-1.363318	1.757925
H	1.908480	-1.431578	1.849202
H	2.745713	0.124626	1.706919

P-H2-6

C	-1.184958	0.550620	0.013373
C	-0.861466	-0.796014	-0.189157
C	-1.840166	-1.772058	-0.107296
C	-3.145850	-1.430199	0.190362
C	-3.467760	-0.099079	0.403738
C	-2.499544	0.885537	0.315487
H	-1.549206	-2.796739	-0.279625
H	-3.905958	-2.191939	0.261005
H	-4.482709	0.176776	0.646360
H	-2.761598	1.914104	0.509713
C	-0.151080	1.557957	-0.107679
C	1.131610	1.241653	-0.278275
C	1.629486	-0.154285	-0.356284
C	0.521608	-1.182068	-0.519206
O	-0.456395	2.886577	0.042368
O	2.103569	2.168249	-0.322983
O	0.803443	-2.300362	-0.882336
H	1.695699	3.029154	-0.197470
H	2.274203	-0.240127	-1.241756
H	-1.151187	3.135986	-0.566218
N	2.348715	-0.463953	0.867655
H	2.833354	0.367997	1.163601
C	3.276169	-1.566914	0.755288
H	3.819883	-1.659682	1.690768
H	3.995674	-1.441987	-0.061683
H	2.737601	-2.492485	0.583214

P-H2-7

C	-1.139504	0.621033	-0.009387
C	-0.980561	-0.766279	-0.124211
C	-2.082978	-1.603402	-0.067881
C	-3.354048	-1.080388	0.073993
C	-3.516452	0.293070	0.172437
C	-2.422443	1.138421	0.135976
H	-1.914458	-2.666658	-0.142623
H	-4.211724	-1.733473	0.103310
H	-4.505952	0.711737	0.276175
H	-2.565298	2.206332	0.195827
C	0.029643	1.473094	-0.014985
C	1.243440	0.994381	-0.289143
C	1.501191	-0.433169	-0.672807
C	0.365326	-1.360114	-0.257526
O	-0.093049	2.827362	0.176277
O	2.330606	1.777755	-0.337238
O	0.557057	-2.538140	-0.092174
H	2.050415	2.678901	-0.155820
H	1.462121	-0.463244	-1.769660
H	-0.539601	3.002800	1.004138
N	2.781326	-0.939324	-0.278153
H	3.499118	-0.387686	-0.716872
C	2.983472	-0.985597	1.151675
H	3.999108	-1.311813	1.353143
H	2.311368	-1.720769	1.585063
H	2.826188	-0.022976	1.650626

P-H2-8

C	-1.121788	0.569988	0.031983
C	-0.818496	-0.767264	-0.256194
C	-1.802134	-1.739698	-0.200018
C	-3.094473	-1.406384	0.161246
C	-3.396828	-0.086800	0.458809
C	-2.424207	0.895865	0.393091
H	-1.527253	-2.753994	-0.446105
H	-3.859240	-2.164984	0.212795
H	-4.401375	0.182111	0.748214
H	-2.671269	1.915341	0.646126
C	-0.087202	1.578998	-0.085987
C	1.196211	1.267849	-0.285002
C	1.662766	-0.142640	-0.334600
C	0.553580	-1.125415	-0.663573
O	-0.400504	2.906233	0.066011
O	2.155578	2.191511	-0.390747
O	0.823616	-2.202431	-1.145036
H	1.750358	3.053637	-0.266917
H	2.432988	-0.239857	-1.098335
H	-1.097811	3.150901	-0.541938
N	2.262265	-0.490365	0.943069
H	1.579915	-0.416290	1.681564
C	2.965384	-1.750834	0.984524
H	3.415049	-1.859754	1.967469
H	3.767643	-1.730832	0.250589
H	2.348737	-2.628212	0.777562

P-H2-9

C	-1.179185	0.569457	0.008546
C	-0.878755	-0.781241	-0.184197
C	-1.876855	-1.737602	-0.096234
C	-3.173722	-1.362934	0.198860
C	-3.472303	-0.022339	0.389991
C	-2.485362	0.942279	0.292072
H	-1.610038	-2.769449	-0.263958
H	-3.949636	-2.108207	0.276588
H	-4.484753	0.275801	0.615854
H	-2.715170	1.985594	0.433962
C	-0.125044	1.564164	-0.104942
C	1.143861	1.217124	-0.306113
C	1.617358	-0.187550	-0.356222
C	0.491183	-1.191861	-0.538131
O	-0.508406	2.848718	0.023358
O	2.090900	2.209874	-0.271712
O	0.748889	-2.306941	-0.927522
H	2.716019	2.100075	-0.987690
H	2.292796	-0.323420	-1.215951
H	0.277784	3.396226	-0.023788
N	2.279954	-0.517744	0.893420
H	2.707941	0.312398	1.268896
C	3.227658	-1.602913	0.807383
H	3.700872	-1.734494	1.775856
H	4.006786	-1.438576	0.053227
H	2.713667	-2.524462	0.553985

P-H2-10

C	-1.112316	0.632944	0.001241
C	-0.980528	-0.749662	-0.183400
C	-2.094842	-1.571681	-0.128646
C	-3.351001	-1.038685	0.086197
C	-3.483572	0.327441	0.281792
C	-2.377186	1.156435	0.248201
H	-1.945174	-2.632757	-0.255479
H	-4.217863	-1.679570	0.113926
H	-4.457626	0.752087	0.471655
H	-2.494380	2.211529	0.441494
C	0.062181	1.475437	-0.058166
C	1.272513	0.979515	-0.317092
C	1.533544	-0.455948	-0.656493
C	0.351452	-1.367479	-0.344255
O	-0.029235	2.821007	0.204893
O	2.366399	1.753361	-0.369279
O	0.507250	-2.559500	-0.260916
H	2.098524	2.652991	-0.162910
H	1.599852	-0.493059	-1.751236
H	-0.655883	3.230764	-0.390827
N	2.763118	-0.983389	-0.141029
H	3.529225	-0.452181	-0.519311
C	2.828183	-1.007853	1.301772
H	3.809277	-1.359358	1.605555
H	2.095732	-1.715642	1.681131
H	2.650618	-0.032805	1.768711

P-H2-11

C	-1.229193	0.594741	-0.038257
C	-1.060443	-0.794807	0.004949
C	-2.161712	-1.634039	-0.024148
C	-3.437680	-1.112220	-0.125464
C	-3.607515	0.262579	-0.182704
C	-2.516872	1.111940	-0.134245
H	-1.988957	-2.697848	0.031005
H	-4.292806	-1.768226	-0.163676
H	-4.599776	0.678860	-0.268098
H	-2.662028	2.179581	-0.195136
C	-0.067649	1.449409	0.064968
C	1.174732	0.965491	0.002730
C	1.474143	-0.484963	-0.247490
C	0.291674	-1.379108	0.132763
O	-0.212163	2.811547	0.166692
O	2.249214	1.761266	0.098245
O	0.455582	-2.524298	0.463091
H	1.931182	2.662705	0.199690
H	1.528082	-0.602421	-1.338526
H	-0.791499	3.025510	0.897642
N	2.703818	-0.971869	0.283728
H	2.809472	-0.738343	1.255468
C	3.896825	-0.702333	-0.479785
H	4.735090	-1.205316	-0.005499
H	4.140099	0.355808	-0.590604
H	3.785478	-1.135491	-1.472487

P-H2-12

C	-1.142100	0.572590	0.020085
C	-0.855148	-0.772608	-0.236096
C	-1.847247	-1.734777	-0.163525
C	-3.136849	-1.382374	0.187516
C	-3.424871	-0.055665	0.462952
C	-2.440795	0.914250	0.379279
H	-1.579927	-2.757009	-0.382637
H	-3.908707	-2.132612	0.253728
H	-4.424996	0.229519	0.751717
H	-2.683825	1.936015	0.627321
C	-0.104622	1.587639	-0.119578
C	1.170598	1.247055	-0.307561
C	1.622939	-0.170681	-0.331779
C	0.511629	-1.163676	-0.611929
O	-0.437403	2.895177	0.014520
O	2.136988	2.193446	-0.331506
O	0.778034	-2.251044	-1.067722
H	2.899267	1.866528	-0.806890
H	2.362273	-0.296355	-1.138456
H	-1.262898	3.065946	-0.436171
N	2.177033	-0.529299	0.961389
H	2.558770	0.286831	1.409575
C	3.124946	-1.616710	0.932272
H	3.497554	-1.787345	1.937726
H	3.976606	-1.432333	0.266657
H	2.634819	-2.524971	0.595544

P-H2-13

C	-1.077177	0.650131	0.027565
C	-1.059920	-0.732764	-0.190593
C	-2.220653	-1.483404	-0.087830
C	-3.415448	-0.876877	0.244963
C	-3.437399	0.489693	0.480825
C	-2.285300	1.247259	0.373490
H	-2.155278	-2.545493	-0.267025
H	-4.318544	-1.459814	0.331231
H	-4.362783	0.971857	0.757258
H	-2.318916	2.303976	0.587601
C	0.126008	1.444864	-0.153794
C	1.311299	0.874558	-0.378261
C	1.495124	-0.606009	-0.400315
C	0.203194	-1.401000	-0.506561
O	0.038628	2.799218	-0.071156
O	2.393515	1.646649	-0.601495
O	0.282726	-2.581024	-0.761531
H	3.142508	1.101392	-0.835001
H	2.087321	-0.848975	-1.298971
H	-0.674562	3.112293	-0.625971
N	2.119678	-1.117221	0.806059
H	2.120083	-2.123397	0.733383
C	3.445673	-0.625600	1.079616
H	3.878190	-1.210407	1.885347
H	3.407165	0.407765	1.411975
H	4.125714	-0.692504	0.216585

P-H3-1

C	-0.469085	1.049426	-0.034119
C	-0.756288	-0.294477	-0.234117
C	-2.082093	-0.697173	-0.258049
C	-3.099168	0.227154	-0.110642
C	-2.806072	1.571841	0.073385
C	-1.490831	1.980210	0.118247
H	-2.313049	-1.746397	-0.370057
H	-4.127022	-0.101352	-0.133351
H	-3.602647	2.290019	0.188268
H	-1.222874	3.013819	0.272594
C	0.921775	1.503239	0.044409
C	1.988180	0.503867	-0.135369
C	1.713399	-0.771905	-0.386393
C	0.329882	-1.333351	-0.436857
H	2.512839	-1.476676	-0.563326
O	1.244116	2.659222	0.244720
O	3.225863	0.997308	-0.053180
H	3.129697	1.944265	0.108234
O	0.221240	-1.925434	-1.705553
N	0.125989	-2.398975	0.528197
H	-0.562708	-2.476988	-1.690469
H	0.817524	-3.109962	0.340119
C	0.164460	-2.011414	1.922024
H	0.090881	-2.905000	2.533809
H	-0.691213	-1.381856	2.150417
H	1.071950	-1.470308	2.203366

P-H3-2

C	-0.572258	0.983485	0.014419
C	-0.767638	-0.364893	-0.258472
C	-2.064242	-0.847391	-0.346597
C	-3.140281	-0.003624	-0.148667
C	-2.938874	1.339211	0.144751
C	-1.655058	1.832603	0.219372
H	-2.223341	-1.885109	-0.598532
H	-4.144361	-0.391177	-0.229830
H	-3.782558	1.993042	0.300290
H	-1.458142	2.873166	0.425409
C	0.781414	1.541202	0.024617
C	1.904505	0.637801	-0.285862
C	1.721139	-0.663680	-0.480399
C	0.388059	-1.333785	-0.398262
H	2.565658	-1.309575	-0.672623
O	1.031351	2.710538	0.249078
O	3.095926	1.237069	-0.330624
H	2.937811	2.169100	-0.133844
O	0.127591	-2.078607	-1.558838
N	0.437341	-2.294593	0.692592
H	0.720849	-2.831310	-1.536862
H	-0.446488	-2.782739	0.703138
C	0.724951	-1.759112	2.005391
H	0.634822	-2.559521	2.733069
H	0.058670	-0.943896	2.304254
H	1.746435	-1.392729	2.038709

P-H3-3

C	-0.517804	1.023461	-0.010691
C	-0.758932	-0.326243	-0.233290
C	-2.066214	-0.780446	-0.290659
C	-3.115520	0.104836	-0.132547
C	-2.872357	1.454848	0.090588
C	-1.574550	1.913857	0.152079
H	-2.235796	-1.832638	-0.457821
H	-4.131590	-0.256222	-0.180669
H	-3.696006	2.140338	0.215074
H	-1.348061	2.954597	0.324071
C	0.856658	1.524541	0.047527
C	1.954466	0.564862	-0.179603
C	1.719349	-0.722814	-0.420329
C	0.353394	-1.338109	-0.413376
H	2.542133	-1.402360	-0.594213
O	1.148040	2.687107	0.257431
O	3.173626	1.105785	-0.139771
H	3.046685	2.045730	0.042452
O	0.169096	-2.054118	-1.614952
N	0.211041	-2.359382	0.595971
H	0.393392	-1.482039	-2.347777
H	0.844864	-3.110477	0.370246
C	0.361484	-1.920738	1.962379
H	0.275982	-2.783876	2.614927
H	-0.445499	-1.237016	2.215427
H	1.310680	-1.418885	2.172358

P-H3-4

C	0.139327	1.151469	0.085654
C	-0.708277	0.100172	-0.254681
C	-2.043254	0.378619	-0.501522
C	-2.526770	1.668456	-0.369595
C	-1.685120	2.704211	0.008677
C	-0.348168	2.445526	0.223324
H	-2.693854	-0.419317	-0.820691
H	-3.568154	1.868674	-0.570831
H	-2.068474	3.707243	0.111094
H	0.347611	3.229812	0.478060
C	1.582536	0.929261	0.189247
C	2.099991	-0.408530	-0.154079
C	1.283440	-1.423615	-0.415866
C	-0.206908	-1.328364	-0.297981
H	1.681856	-2.402513	-0.637763
O	2.384434	1.792781	0.492133
O	3.431329	-0.498318	-0.165722
H	3.763240	0.374798	0.079017
O	-0.843776	-1.930086	-1.392815
N	-0.542690	-2.104997	0.885080
H	-0.694052	-2.872991	-1.309834
H	0.092320	-1.888633	1.634963
C	-1.917452	-2.110989	1.328275
H	-2.023073	-2.858985	2.108747
H	-2.559188	-2.403764	0.501734
H	-2.271358	-1.151666	1.712458

P-H3-5

C	1.195043	0.471462	-0.035327
C	0.475341	-0.708844	0.107991
C	1.163438	-1.912748	0.100564
C	2.539868	-1.935222	-0.028972
C	3.253094	-0.752090	-0.160809
C	2.578354	0.449716	-0.168672
H	0.612081	-2.837613	0.180867
H	3.060202	-2.880808	-0.030050
H	4.326833	-0.773731	-0.261367
H	3.095742	1.390040	-0.278679
C	0.501444	1.761621	-0.066255
C	-0.961485	1.761963	0.085368
C	-1.648481	0.638429	0.262324
C	-1.031383	-0.724160	0.279694
H	-2.714309	0.682148	0.423744
O	1.068679	2.828954	-0.206607
O	-1.519062	2.975108	0.049795
H	-0.795076	3.602636	-0.067813
O	-1.383934	-1.255198	1.534628
N	-1.557100	-1.618887	-0.734535
H	-1.184056	-2.192143	1.506947
H	-1.100996	-1.451558	-1.616591
C	-2.996796	-1.645794	-0.878803
H	-3.273628	-2.504145	-1.483872
H	-3.417035	-0.748963	-1.338905
H	-3.446144	-1.770562	0.102322

P-H3-6

C	1.136617	0.555954	-0.107275
C	0.536663	-0.671894	0.144747
C	1.336325	-1.798224	0.256265
C	2.705977	-1.702355	0.089650
C	3.297987	-0.477434	-0.185757
C	2.513004	0.652305	-0.274635
H	0.878447	-2.746030	0.497484
H	3.317954	-2.586678	0.181594
H	4.366588	-0.408008	-0.315116
H	2.939103	1.625125	-0.464773
C	0.327624	1.775166	-0.127801
C	-1.105994	1.657343	0.198091
C	-1.686906	0.478855	0.400026
C	-0.965822	-0.824475	0.254090
H	-2.736816	0.428030	0.644688
O	0.775540	2.884012	-0.350831
O	-1.747278	2.824379	0.277878
H	-1.096029	3.505853	0.067868
O	-1.280276	-1.654564	1.367337
N	-1.400933	-1.488086	-0.937713
H	-1.088404	-1.184015	2.178106
H	-0.857716	-2.327670	-1.058969
C	-2.817227	-1.774999	-1.028583
H	-2.979242	-2.423295	-1.883964
H	-3.370969	-0.858349	-1.212693
H	-3.219769	-2.260430	-0.138221

P-H3-7

C	1.197097	0.464940	-0.063151
C	0.472531	-0.708320	0.109953
C	1.145936	-1.918991	0.150317
C	2.521310	-1.953268	0.018373
C	3.242740	-0.779194	-0.159133
C	2.581065	0.428883	-0.198820
H	0.570816	-2.820830	0.288819
H	3.037647	-2.900477	0.053652
H	4.316008	-0.813211	-0.262652
H	3.108514	1.360588	-0.331691
C	0.510819	1.757748	-0.087799
C	-0.949710	1.767160	0.110221
C	-1.642686	0.644686	0.286282
C	-1.034022	-0.725948	0.257537
H	-2.709977	0.693847	0.442906
O	1.075035	2.823848	-0.249100
O	-1.496531	2.984955	0.102695
H	-0.771188	3.606098	-0.041403
O	-1.394422	-1.403380	1.444927
N	-1.552467	-1.561999	-0.797474
H	-1.228609	-0.824827	2.187991
H	-1.141486	-1.294526	-1.676154
C	-2.991122	-1.668748	-0.884209
H	-3.237990	-2.465330	-1.579875
H	-3.494962	-0.756922	-1.215602
H	-3.377917	-1.947493	0.090716

P-H3-8

C	-0.479720	1.021983	0.002340
C	-0.761889	-0.313424	-0.259030
C	-2.088052	-0.708242	-0.349883
C	-3.107006	0.209427	-0.177037
C	-2.817811	1.540710	0.094784
C	-1.503954	1.946460	0.180080
H	-2.314559	-1.740897	-0.571073
H	-4.134407	-0.112070	-0.255460
H	-3.616695	2.252485	0.231264
H	-1.239231	2.973596	0.377659
C	0.910605	1.481936	0.045461
C	1.976070	0.497924	-0.222883
C	1.707350	-0.787572	-0.434145
C	0.329851	-1.365218	-0.393384
H	2.498058	-1.501703	-0.605457
O	1.234840	2.633299	0.267119
O	3.207950	1.010903	-0.226791
H	3.111566	1.952010	-0.034163
O	0.090240	-2.133358	-1.549843
N	0.283462	-2.348235	0.663033
H	0.109039	-1.556404	-2.311907
H	-0.516572	-2.940928	0.502984
C	0.309102	-1.832658	2.009373
H	0.294125	-2.668367	2.701953
H	-0.523851	-1.165143	2.252425
H	1.236765	-1.289633	2.172618

P-H3-9

C	-0.197090	1.153152	-0.103515
C	0.705323	0.140439	0.209660
C	2.026327	0.480096	0.454573
C	2.444520	1.795306	0.346050
C	1.547865	2.793579	-0.003577
C	0.223472	2.471819	-0.216114
H	2.721447	-0.293088	0.742265
H	3.476971	2.043090	0.540208
H	1.879179	3.816597	-0.088426
H	-0.511464	3.225084	-0.453872
C	-1.627613	0.858384	-0.210080
C	-2.078622	-0.500339	0.142510
C	-1.212421	-1.473664	0.402135
C	0.269529	-1.311013	0.260839
H	-1.558380	-2.467861	0.645984
O	-2.470762	1.682207	-0.510151
O	-3.403471	-0.650242	0.173483
H	-3.777769	0.202502	-0.082219
O	0.920037	-1.967624	1.339402
N	0.635663	-1.966882	-0.960766
H	0.665762	-1.550301	2.161985
H	0.164749	-2.855888	-0.998837
C	2.046055	-2.131003	-1.239959
H	2.144213	-2.817619	-2.075123
H	2.614429	-2.525358	-0.395709
H	2.480718	-1.184237	-1.547906

P-H3-10

C	0.219939	1.150979	0.087505
C	-0.696787	0.149405	-0.226459
C	-2.018016	0.509686	-0.450045
C	-2.418401	1.828606	-0.323500
C	-1.505703	2.813717	0.023178
C	-0.182974	2.473961	0.216859
H	-2.727621	-0.250193	-0.737457
H	-3.450282	2.090424	-0.501859
H	-1.823860	3.839731	0.120682
H	0.564187	3.216347	0.450992
C	1.647341	0.835897	0.183598
C	2.074072	-0.540090	-0.132445
C	1.193400	-1.505998	-0.377864
C	-0.286940	-1.314498	-0.275211
H	1.512588	-2.517249	-0.576573
O	2.504531	1.652284	0.464531
O	3.396587	-0.717179	-0.138947
H	3.785806	0.135593	0.092356
O	-0.940318	-1.947693	-1.349144
N	-0.693583	-2.060186	0.892903
H	-0.727277	-1.478970	-2.154653
H	-0.127034	-1.795962	1.680335
C	-2.097582	-2.111317	1.217824
H	-2.238437	-2.849354	2.002337
H	-2.647922	-2.448520	0.344761
H	-2.521544	-1.161932	1.556611

P-H3-11

C	-0.174086	1.155962	-0.096789
C	0.708840	0.131320	0.228987
C	2.034875	0.446561	0.475584
C	2.476625	1.752535	0.355525
C	1.600505	2.764443	-0.008110
C	0.271602	2.465778	-0.221605
H	2.711949	-0.334700	0.781546
H	3.512061	1.983630	0.554345
H	1.951476	3.780140	-0.101610
H	-0.448796	3.230044	-0.468384
C	-1.608145	0.887341	-0.204477
C	-2.084960	-0.462327	0.151480
C	-1.236576	-1.448969	0.413231
C	0.247618	-1.308392	0.273022
H	-1.614518	-2.433232	0.657018
O	-2.438371	1.722711	-0.509460
O	-3.412149	-0.588616	0.180030
H	-3.769104	0.271924	-0.075329
O	0.902292	-1.873977	1.394622
N	0.592225	-1.953709	-0.968361
H	0.616230	-2.781192	1.493256
H	0.049297	-2.791124	-1.093785
C	1.989954	-2.163710	-1.265093
H	2.061047	-2.839076	-2.111967
H	2.555674	-2.587585	-0.432154
H	2.457412	-1.227054	-1.556477

P-H3-12

C	1.162508	0.513669	-0.070934
C	0.500266	-0.690866	0.128048
C	1.251408	-1.856126	0.178512
C	2.626062	-1.820980	0.033612
C	3.277975	-0.613634	-0.169053
C	2.543554	0.551482	-0.219726
H	0.769571	-2.813402	0.330832
H	3.191431	-2.739039	0.079399
H	4.350153	-0.587411	-0.282537
H	3.012700	1.511247	-0.370924
C	0.412910	1.772520	-0.102217
C	-1.035991	1.718511	0.136597
C	-1.673399	0.569970	0.328271
C	-1.006591	-0.766066	0.260791
H	-2.729580	0.568015	0.546662
O	0.931486	2.857824	-0.285885
O	-1.636135	2.911850	0.164300
H	-0.946562	3.566374	-0.000868
O	-1.362985	-1.382567	1.490494
N	-1.485161	-1.478512	-0.892030
H	-0.867159	-2.192849	1.598459
H	-0.937247	-2.306693	-1.053355
C	-2.903205	-1.756922	-0.940879
H	-3.090990	-2.446009	-1.758194
H	-3.455620	-0.846474	-1.156854
H	-3.292478	-2.190382	-0.017811

P-H3-13

C	-0.519614	1.029706	-0.031641
C	-0.744100	-0.323566	-0.238288
C	-2.048136	-0.793532	-0.274765
C	-3.111470	0.076910	-0.133832
C	-2.883703	1.433079	0.057274
C	-1.590089	1.905019	0.114714
H	-2.224501	-1.853065	-0.390644
H	-4.121778	-0.301360	-0.166550
H	-3.714435	2.112400	0.167725
H	-1.373624	2.949733	0.274732
C	0.848474	1.579091	0.061128
C	1.962374	0.622138	-0.130423
C	1.737332	-0.666326	-0.373103
C	0.389262	-1.307224	-0.428429
H	2.562289	-1.344822	-0.553276
O	1.062263	2.747439	0.275630
O	3.167124	1.203137	-0.054537
H	3.853156	0.559533	-0.222856
O	0.329747	-1.912268	-1.695101
N	0.236506	-2.377764	0.539699
H	-0.437750	-2.486545	-1.695628
H	0.960924	-3.056831	0.358509
C	0.241351	-1.983864	1.931762
H	0.209971	-2.877637	2.546987
H	-0.648258	-1.399427	2.149314
H	1.115306	-1.392681	2.219480

P-H3-14

C	-0.601717	0.965809	0.006404
C	-0.759484	-0.386183	-0.265061
C	-2.039836	-0.909565	-0.365403
C	-3.143000	-0.098397	-0.183715
C	-2.981732	1.250099	0.107278
C	-1.713240	1.780072	0.196358
H	-2.163475	-1.953008	-0.614026
H	-4.134390	-0.515278	-0.274952
H	-3.844980	1.881029	0.250491
H	-1.547789	2.825862	0.403325
C	0.735120	1.590838	0.044568
C	1.883978	0.716363	-0.290538
C	1.728832	-0.591627	-0.475111
C	0.425303	-1.316807	-0.381758
H	2.583981	-1.224482	-0.678615
O	0.899736	2.756184	0.312184
O	3.043843	1.382554	-0.356551
H	3.754159	0.784702	-0.583097
O	0.207093	-2.096226	-1.528443
N	0.509916	-2.256265	0.726688
H	0.801149	-2.845771	-1.462497
H	-0.352047	-2.782784	0.734152
C	0.744141	-1.681736	2.034105
H	0.694645	-2.474028	2.774453
H	0.024097	-0.905248	2.308535
H	1.739682	-1.250423	2.075129

P-H3-15

C	-0.565301	1.003430	-0.011816
C	-0.748750	-0.354488	-0.232196
C	-2.033678	-0.870790	-0.291625
C	-3.123718	-0.036229	-0.138952
C	-2.940558	1.323510	0.081041
C	-1.664800	1.840897	0.145537
H	-2.152495	-1.930587	-0.455438
H	-4.121982	-0.443740	-0.188534
H	-3.794157	1.972274	0.201685
H	-1.485693	2.890777	0.317400
C	0.784673	1.597088	0.062115
C	1.926237	0.679631	-0.170078
C	1.737596	-0.617771	-0.406819
C	0.407853	-1.309917	-0.409872
H	2.583036	-1.272191	-0.586011
O	0.967429	2.768902	0.286663
O	3.111346	1.302683	-0.128208
H	3.817697	0.676306	-0.276661
O	0.276365	-2.027633	-1.617892
N	0.317752	-2.344905	0.590161
H	0.381445	-1.417691	-2.346898
H	0.982698	-3.066454	0.358092
C	0.445230	-1.910761	1.959815
H	0.398219	-2.781596	2.606064
H	-0.392167	-1.265932	2.215296
H	1.369295	-1.366052	2.176481

P-H3-16

C	1.172302	0.534889	-0.040135
C	0.519089	-0.680232	0.115584
C	1.265980	-1.849297	0.121675
C	2.641225	-1.805166	-0.006447
C	3.290945	-0.587551	-0.151851
C	2.555287	0.577796	-0.173269
H	0.761147	-2.799832	0.210040
H	3.209432	-2.722694	0.003293
H	4.364522	-0.553473	-0.252115
H	3.023155	1.542447	-0.293426
C	0.429809	1.810726	-0.083995
C	-1.037259	1.727627	0.089226
C	-1.655552	0.562624	0.261864
C	-0.982327	-0.772938	0.276342
H	-2.723280	0.535230	0.433502
O	0.980037	2.872781	-0.246364
O	-1.632290	2.928231	0.066669
H	-2.570636	2.831770	0.219544
O	-1.327151	-1.322376	1.526189
N	-1.457587	-1.686490	-0.745330
H	-1.060913	-2.242860	1.509838
H	-0.999655	-1.497532	-1.621876
C	-2.891124	-1.786850	-0.902279
H	-3.118849	-2.651051	-1.519447
H	-3.355299	-0.908552	-1.357699
H	-3.341532	-1.946879	0.073405

P-H3-17

C	0.017278	1.161773	0.078614
C	-0.717931	0.031796	-0.264062
C	-2.073056	0.167054	-0.523912
C	-2.688272	1.400583	-0.408183
C	-1.958708	2.517731	-0.029736
C	-0.604784	2.397456	0.203437
H	-2.634548	-0.698324	-0.837301
H	-3.742670	1.491918	-0.620256
H	-2.442229	3.477819	0.061114
H	0.003871	3.248958	0.465051
C	1.485237	1.108894	0.224904
C	2.137967	-0.165030	-0.162736
C	1.420992	-1.255447	-0.419988
C	-0.069329	-1.333408	-0.287259
H	1.905448	-2.191462	-0.666867
O	2.138768	2.052324	0.598547
O	3.473672	-0.077092	-0.202698
H	3.851554	-0.917771	-0.455237
O	-0.634021	-2.026889	-1.367551
N	-0.309342	-2.125094	0.909997
H	-0.417712	-2.951396	-1.237454
H	0.293389	-1.813449	1.653358
C	-1.676586	-2.262540	1.359226
H	-1.705406	-3.004279	2.152147
H	-2.288211	-2.630008	0.539685
H	-2.122300	-1.336263	1.727565

P-H3-18

C	1.122362	0.595327	-0.101573
C	0.565859	-0.652379	0.143444
C	1.398609	-1.755016	0.258829
C	2.765861	-1.616282	0.106691
C	3.317665	-0.371244	-0.159988
C	2.496279	0.732270	-0.256350
H	0.967250	-2.717895	0.489960
H	3.405181	-2.480667	0.201970
H	4.384622	-0.265246	-0.278793
H	2.891027	1.718487	-0.444821
C	0.286730	1.810940	-0.150025
C	-1.143822	1.641469	0.199534
C	-1.676888	0.437892	0.394505
C	-0.928715	-0.849887	0.241857
H	-2.722201	0.336791	0.654883
O	0.736115	2.897877	-0.419901
O	-1.795908	2.807151	0.294817
H	-2.719548	2.653083	0.485527
O	-1.232078	-1.686817	1.354394
N	-1.349616	-1.521000	-0.950200
H	-0.972235	-1.243888	2.161769
H	-0.775303	-2.337736	-1.083157
C	-2.753999	-1.860422	-1.031965
H	-2.900249	-2.504538	-1.893307
H	-3.343807	-0.963350	-1.202735
H	-3.132106	-2.369735	-0.144123

P-H3-19

C	-0.519905	1.008551	-0.003970
C	-0.750684	-0.336720	-0.258228
C	-2.058668	-0.790248	-0.350360
C	-3.116769	0.083027	-0.188214
C	-2.881589	1.426314	0.074909
C	-1.585535	1.886525	0.163566
H	-2.239376	-1.834081	-0.562076
H	-4.129568	-0.281717	-0.266988
H	-3.708871	2.106587	0.203697
H	-1.363886	2.924392	0.357828
C	0.852360	1.553118	0.061051
C	1.957134	0.602775	-0.209560
C	1.727812	-0.691819	-0.418201
C	0.381497	-1.338603	-0.388056
H	2.538539	-1.386749	-0.592091
O	1.075889	2.713835	0.304649
O	3.160666	1.190590	-0.209698
H	3.842055	0.540226	-0.372078
O	0.194428	-2.110732	-1.552584
N	0.382454	-2.331617	0.660553
H	0.099776	-1.520357	-2.298599
H	-0.377416	-2.970500	0.483168
C	0.349375	-1.822362	2.009638
H	0.391668	-2.659519	2.699441
H	-0.536146	-1.223020	2.242181
H	1.228014	-1.206842	2.187271

P-H3-20

C	1.177959	0.522451	-0.061201
C	0.512247	-0.683574	0.111447
C	1.238033	-1.864294	0.155566
C	2.613339	-1.838525	0.027652
C	3.278790	-0.632047	-0.149874
C	2.562400	0.544470	-0.193506
H	0.702409	-2.790530	0.292086
H	3.172233	-2.761131	0.065310
H	4.352836	-0.615420	-0.251009
H	3.046052	1.499401	-0.327781
C	0.450396	1.806193	-0.099526
C	-1.015646	1.740940	0.106778
C	-1.646260	0.580087	0.279403
C	-0.988838	-0.768650	0.252652
H	-2.716228	0.563515	0.443781
O	1.006245	2.862912	-0.277310
O	-1.594739	2.949327	0.101824
H	-2.538043	2.862047	0.227761
O	-1.333203	-1.455005	1.440236
N	-1.472391	-1.625006	-0.801566
H	-1.103565	-0.903368	2.186731
H	-1.072074	-1.341815	-1.680023
C	-2.902880	-1.802039	-0.887297
H	-3.111975	-2.603447	-1.589797
H	-3.453560	-0.914203	-1.211937
H	-3.275003	-2.107942	0.085277

P-H3-21

C	0.073203	1.170995	0.097181
C	-0.718267	0.070913	-0.212914
C	-2.067589	0.263961	-0.466368
C	-2.624244	1.527655	-0.374409
C	-1.837893	2.616060	-0.029564
C	-0.488511	2.436631	0.196353
H	-2.675683	-0.583147	-0.743911
H	-3.676008	1.663336	-0.575330
H	-2.274214	3.599949	0.043974
H	0.161286	3.263613	0.436966
C	1.537852	1.049145	0.241832
C	2.129284	-0.253475	-0.146100
C	1.361144	-1.308489	-0.402563
C	-0.129074	-1.322242	-0.250974
H	1.796360	-2.263514	-0.670653
O	2.234338	1.965362	0.604212
O	3.466700	-0.225398	-0.198630
H	3.806593	-1.092552	-0.412459
O	-0.696263	-2.058090	-1.326808
N	-0.413530	-2.013815	0.972056
H	-0.563904	-1.575551	-2.142425
H	0.137005	-2.856469	0.997552
C	-1.798922	-2.309542	1.267399
H	-1.823465	-2.999525	2.105241
H	-2.336891	-2.757901	0.430055
H	-2.316448	-1.406206	1.577171

P-H3-22

C	0.109849	1.172547	0.081499
C	-0.710247	0.091436	-0.228258
C	-2.060203	0.319932	-0.456201
C	-2.585861	1.594962	-0.342754
C	-1.769460	2.662644	-0.001809
C	-0.421282	2.450215	0.200454
H	-2.693598	-0.508504	-0.733143
H	-3.637504	1.756541	-0.524392
H	-2.181879	3.655471	0.087241
H	0.251438	3.260314	0.435740
C	1.573440	1.014979	0.208680
C	2.125574	-0.317267	-0.134711
C	1.329260	-1.355808	-0.377604
C	-0.162425	-1.322654	-0.266875
H	1.728602	-2.337572	-0.593029
O	2.297677	1.922150	0.539115
O	3.464500	-0.337842	-0.155907
H	3.775277	-1.219055	-0.357117
O	-0.743187	-2.029253	-1.337088
N	-0.483038	-2.104309	0.905596
H	-0.651544	-1.505406	-2.131541
H	0.043124	-1.761025	1.691068
C	-1.875659	-2.297815	1.230211
H	-1.940940	-3.037250	2.023293
H	-2.386299	-2.699570	0.360490
H	-2.395245	-1.393247	1.557475

P-H3-23

C	1.144600	0.562798	-0.070912
C	0.534675	-0.667044	0.129261
C	1.328665	-1.804100	0.188985
C	2.701701	-1.716978	0.055096
C	3.304328	-0.484645	-0.147913
C	2.524105	0.650136	-0.210426
H	0.880843	-2.778609	0.338057
H	3.302546	-2.611809	0.108306
H	4.375476	-0.414901	-0.253663
H	2.955034	1.627093	-0.364841
C	0.360085	1.813868	-0.124071
C	-1.089548	1.695279	0.137611
C	-1.671444	0.515064	0.321136
C	-0.965778	-0.800221	0.249929
H	-2.726266	0.455041	0.551495
O	0.872985	2.884369	-0.342876
O	-1.709011	2.883467	0.181554
H	-2.639823	2.761342	0.359311
O	-1.313843	-1.431952	1.475852
N	-1.416511	-1.526120	-0.906012
H	-0.740015	-2.181929	1.624165
H	-0.830931	-2.327002	-1.072670
C	-2.818809	-1.872596	-0.947785
H	-2.980015	-2.561753	-1.770709
H	-3.417001	-0.988250	-1.152575
H	-3.180799	-2.332812	-0.026495

P-H3-24

C	0.029510	1.168502	0.092055
C	-0.722498	0.049506	-0.243691
C	-2.073901	0.199299	-0.509114
C	-2.671341	1.442988	-0.404633
C	-1.925903	2.551735	-0.033807
C	-0.574261	2.413645	0.204758
H	-2.647234	-0.661400	-0.814542
H	-3.723950	1.548042	-0.619206
H	-2.395498	3.519495	0.048648
H	0.045363	3.257782	0.464363
C	1.494425	1.091474	0.248192
C	2.131961	-0.182388	-0.166552
C	1.400453	-1.260081	-0.431063
C	-0.087721	-1.320439	-0.264977
H	1.879259	-2.189670	-0.718861
O	2.161064	2.018945	0.637254
O	3.466572	-0.101587	-0.231954
H	3.837475	-0.943697	-0.489281
O	-0.670603	-1.993228	-1.367509
N	-0.331388	-1.981889	0.990841
H	-0.346240	-2.892752	-1.383937
H	0.306286	-2.749169	1.120018
C	-1.691226	-2.340075	1.319699
H	-1.673199	-2.983806	2.193601
H	-2.217603	-2.858616	0.514684
H	-2.258190	-1.451015	1.581106

P-H4-1

C	0.712922	-0.727219	-0.208559
C	1.274062	0.531567	0.015016
C	2.627929	0.628204	0.296050
C	3.402902	-0.517079	0.365751
C	2.844009	-1.764451	0.137070
C	1.498527	-1.865744	-0.163630
H	3.065763	1.600102	0.453133
H	4.454536	-0.433343	0.593244
H	3.456239	-2.651069	0.188623
H	1.034492	-2.819037	-0.363733
C	-0.709443	-0.827752	-0.558069
C	-1.611258	0.343466	-0.186721
C	-0.889794	1.647608	-0.239873
C	0.430943	1.721768	-0.102386
H	-1.505972	2.528006	-0.357087
O	-1.201255	-1.807839	-1.070614
O	1.132718	2.874003	-0.073962
H	0.539953	3.619990	-0.143762
O	-2.689275	0.388084	-1.070565
N	-1.980475	0.072819	1.185199
H	-2.811241	-0.505396	-1.405740
H	-2.237134	0.931367	1.642947
C	-2.977552	-0.954590	1.387116
H	-3.158378	-1.054354	2.453063
H	-2.607373	-1.910734	1.026339
H	-3.924551	-0.743907	0.887122

P-H4-2

C	-0.907202	-0.733784	0.074342
C	-1.176357	0.636259	0.056212
C	-2.474251	1.065440	-0.178434
C	-3.479178	0.140155	-0.400259
C	-3.209166	-1.219777	-0.376426
C	-1.922046	-1.654920	-0.128077
H	-2.687228	2.121519	-0.181373
H	-4.484633	0.484249	-0.588539
H	-3.999824	-1.933140	-0.548032
H	-1.676413	-2.704845	-0.091151
C	0.452587	-1.198686	0.354512
C	1.602072	-0.201824	0.264858
C	1.172319	1.212840	0.451130
C	-0.097396	1.585822	0.325056
H	1.949091	1.925914	0.686658
O	0.729306	-2.352771	0.597668
O	-0.532247	2.858517	0.446544
H	0.205969	3.441005	0.614872
O	2.539753	-0.494215	1.265038
N	2.093806	-0.422371	-1.071308
H	2.534172	-1.449345	1.374249
H	2.346639	-1.395722	-1.158197
C	3.183894	0.433536	-1.483758
H	3.568634	0.075204	-2.433477
H	4.003282	0.464919	-0.762116
H	2.817525	1.444210	-1.642682

P-H4-3

C	-0.684945	-0.721079	0.226118
C	-1.265733	0.529718	0.000114
C	-2.622435	0.604000	-0.275727
C	-3.380138	-0.553650	-0.335110
C	-2.802120	-1.792139	-0.104613
C	-1.453626	-1.872032	0.189077
H	-3.075476	1.568409	-0.435818
H	-4.434303	-0.486343	-0.556337
H	-3.402155	-2.687458	-0.147630
H	-0.973797	-2.816605	0.393864
C	0.739053	-0.791851	0.580752
C	1.621940	0.386563	0.193907
C	0.886557	1.681049	0.223458
C	-0.436026	1.733644	0.092835
H	1.497782	2.569603	0.278036
O	1.250287	-1.770904	1.079711
O	-1.154122	2.875244	0.029432
H	-0.570665	3.630337	0.078525
O	2.709209	0.427913	1.049727
N	2.075793	0.162189	-1.171096
H	2.802384	-0.455023	1.420924
H	1.319119	0.290692	-1.822721
C	2.840588	-1.035989	-1.422693
H	3.196769	-1.005324	-2.448197
H	2.296836	-1.972292	-1.268728
H	3.711274	-1.038742	-0.773910

P-H4-4

C	0.705394	-0.729849	-0.223801
C	1.077346	0.612902	-0.121497
C	2.412370	0.930133	0.084329
C	3.353772	-0.077813	0.196311
C	2.982241	-1.409740	0.091056
C	1.657034	-1.732656	-0.127612
H	2.703134	1.965499	0.149413
H	4.388874	0.179184	0.361554
H	3.723816	-2.188478	0.175574
H	1.332021	-2.756940	-0.225500
C	-0.700892	-1.080739	-0.458422
C	-1.773714	-0.002856	-0.260329
C	-1.232628	1.380241	-0.398698
C	0.063474	1.655823	-0.275045
H	-1.967197	2.162530	-0.534862
O	-1.059911	-2.187359	-0.779122
O	0.585320	2.902072	-0.296916
H	-0.111478	3.545466	-0.411526
O	-2.762502	-0.169611	-1.218240
N	-2.374074	-0.250397	1.040634
H	-2.986312	-1.104868	-1.204163
H	-3.130925	0.407414	1.151467
C	-1.487579	-0.227977	2.180408
H	-2.083681	-0.276269	3.086095
H	-0.848707	0.659620	2.232998
H	-0.845183	-1.106004	2.168539

P-H4-5

C	0.696057	-0.734008	-0.214997
C	1.087316	0.604297	-0.124886
C	2.426554	0.902438	0.077622
C	3.352611	-0.119595	0.196800
C	2.961840	-1.446656	0.103190
C	1.631746	-1.751162	-0.112311
H	2.733266	1.933554	0.135837
H	4.391584	0.123183	0.359306
H	3.692083	-2.235398	0.192947
H	1.291490	-2.771074	-0.203535
C	-0.711712	-1.055964	-0.463530
C	-1.770251	0.034415	-0.263845
C	-1.215414	1.410987	-0.365035
C	0.086475	1.662682	-0.271887
H	-1.947388	2.200011	-0.457313
O	-1.091676	-2.164795	-0.772524
O	0.628433	2.899544	-0.296916
H	-0.060819	3.554706	-0.390012
O	-2.742522	-0.141446	-1.240449
N	-2.402011	-0.135448	1.035268
H	-2.760622	-1.081293	-1.445380
H	-2.987940	-0.955468	0.985185
C	-1.536573	-0.181822	2.191700
H	-2.150395	-0.183427	3.087560
H	-0.921195	0.713897	2.218202
H	-0.871762	-1.050655	2.232521

P-H4-6

C	0.898586	-0.738442	-0.100779
C	1.157766	0.634581	-0.084576
C	2.444536	1.074705	0.187513
C	3.446897	0.157663	0.454262
C	3.186445	-1.203886	0.435140
C	1.911390	-1.650823	0.144076
H	2.651744	2.132060	0.181769
H	4.443390	0.510018	0.672404
H	3.975334	-1.910237	0.640500
H	1.675414	-2.702952	0.102562
C	-0.453620	-1.207803	-0.434373
C	-1.607513	-0.225387	-0.240576
C	-1.189426	1.184467	-0.521472
C	0.077698	1.571742	-0.398838
H	-1.973220	1.884816	-0.772075
O	-0.694989	-2.329752	-0.804333
O	0.510273	2.842495	-0.551515
H	-0.227430	3.416220	-0.750059
O	-2.637744	-0.546372	-1.108158
N	-2.047239	-0.452660	1.129320
H	-2.695232	-1.506575	-1.110083
H	-1.261032	-0.394424	1.759169
C	-3.114148	0.421276	1.565829
H	-3.465439	0.087771	2.537758
H	-3.938389	0.338826	0.864209
H	-2.826451	1.473559	1.643425

P-H4-7

C	0.699748	-0.717195	-0.254820
C	1.258326	0.535662	0.014518
C	2.600577	0.604866	0.356979
C	3.370555	-0.546058	0.411762
C	2.815998	-1.779151	0.115711
C	1.476833	-1.860148	-0.222479
H	3.051124	1.551956	0.613619
H	4.410909	-0.475757	0.689580
H	3.421338	-2.670850	0.155795
H	1.010445	-2.804486	-0.457193
C	-0.726442	-0.805740	-0.600819
C	-1.617334	0.353632	-0.171903
C	-0.897881	1.658160	-0.247945
C	0.421730	1.732825	-0.120109
H	-1.495190	2.546716	-0.377593
O	-1.220707	-1.770376	-1.138028
O	1.030914	2.941328	-0.087068
H	1.905582	2.879750	-0.467301
O	-2.732489	0.405897	-1.006033
N	-1.920310	0.063798	1.211499
H	-2.856681	-0.478261	-1.363836
H	-2.159037	0.915292	1.691935
C	-2.904071	-0.970424	1.441606
H	-3.028863	-1.096127	2.512803
H	-2.551577	-1.917035	1.039425
H	-3.875875	-0.751143	0.996286

P-H4-8

C	-0.888344	-0.738208	0.117028
C	-1.149849	0.634536	0.073411
C	-2.436778	1.054420	-0.232335
C	-3.439731	0.128340	-0.467228
C	-3.177966	-1.229554	-0.394089
C	-1.897692	-1.659785	-0.098796
H	-2.660952	2.106786	-0.320026
H	-4.432605	0.472761	-0.712429
H	-3.964170	-1.945124	-0.575561
H	-1.653466	-2.709204	-0.040454
C	0.473380	-1.201673	0.404429
C	1.616435	-0.206195	0.253216
C	1.191033	1.200672	0.505831
C	-0.076044	1.579529	0.392458
H	1.952141	1.913747	0.778206
O	0.744314	-2.349163	0.678762
O	-0.405075	2.884985	0.547834
H	-1.271236	2.961569	0.944397
O	2.622255	-0.516518	1.175139
N	2.006082	-0.391948	-1.121380
H	2.597029	-1.469475	1.299662
H	2.280589	-1.355210	-1.246201
C	3.038714	0.502872	-1.598314
H	3.338723	0.190114	-2.593605
H	3.920312	0.523146	-0.954119
H	2.640173	1.510382	-1.677771

P-H4-9

C	0.940445	-0.730099	0.076284
C	1.255300	0.629087	0.049601
C	2.584530	1.017988	-0.024438
C	3.581324	0.059400	-0.084638
C	3.266338	-1.290188	-0.058103
C	1.944124	-1.682606	0.032517
H	2.827725	2.067675	-0.029557
H	4.613036	0.369647	-0.147610
H	4.049610	-2.030515	-0.102695
H	1.663020	-2.723466	0.071262
C	-0.463757	-1.158410	0.205580
C	-1.551232	-0.137432	-0.143175
C	-1.111997	1.272881	0.073488
C	0.174772	1.612396	0.129082
H	-1.883789	2.025718	0.144066
O	-0.766038	-2.288125	0.497502
O	0.621107	2.877719	0.268642
H	-0.116865	3.482165	0.323788
O	-1.786325	-0.355252	-1.542309
N	-2.700763	-0.465049	0.611770
H	-1.272728	0.273382	-2.047399
H	-2.771135	-1.469978	0.658740
C	-3.939810	0.147178	0.197749
H	-4.743084	-0.260050	0.803790
H	-4.173236	-0.014355	-0.855132
H	-3.917388	1.219214	0.383985

P-H4-10

C	0.668738	-0.709543	-0.273225
C	1.249332	0.533639	0.000654
C	2.595510	0.577824	0.334171
C	3.346340	-0.586364	0.373956
C	2.769911	-1.809115	0.075139
C	1.427093	-1.866107	-0.252990
H	3.062651	1.516271	0.591911
H	4.390260	-0.534637	0.642452
H	3.361768	-2.710230	0.103536
H	0.942771	-2.800137	-0.493136
C	-0.759313	-0.765156	-0.621581
C	-1.629081	0.400818	-0.173177
C	-0.894246	1.695929	-0.219634
C	0.428041	1.746509	-0.104457
H	-1.484070	2.595048	-0.288977
O	-1.275500	-1.728417	-1.144061
O	1.057909	2.944351	-0.030612
H	1.907751	2.897116	-0.465531
O	-2.750830	0.455854	-0.981306
N	-2.019266	0.146004	1.204085
H	-2.848974	-0.413816	-1.380931
H	-1.245798	0.290668	1.831599
C	-2.751184	-1.069096	1.467820
H	-3.070434	-1.058740	2.505712
H	-2.195873	-1.993169	1.281744
H	-3.644673	-1.080744	0.850798

P-H4-11

C	0.725319	-0.723072	-0.180826
C	1.302520	0.531808	0.016154
C	2.667104	0.627483	0.245977
C	3.442419	-0.518116	0.286320
C	2.869331	-1.764626	0.088073
C	1.512182	-1.863000	-0.153136
H	3.110947	1.599065	0.387246
H	4.502919	-0.436186	0.468932
H	3.480155	-2.653335	0.117515
H	1.034759	-2.814797	-0.326948
C	-0.716941	-0.853314	-0.475340
C	-1.620303	0.360839	-0.231053
C	-0.866557	1.649991	-0.168988
C	0.455689	1.721030	-0.043822
H	-1.471577	2.545955	-0.203079
O	-1.199760	-1.905062	-0.812051
O	1.150746	2.874557	0.042990
H	0.555795	3.620147	-0.010909
O	-2.552220	0.364214	-1.267647
N	-2.326905	0.208239	1.024507
H	-3.298716	0.878903	-0.958299
H	-1.750913	0.495462	1.797724
C	-3.010762	-1.045698	1.264953
H	-3.710396	-0.905205	2.084264
H	-2.347901	-1.879544	1.501986
H	-3.566867	-1.317755	0.373817

P-H4-12

C	0.690653	-0.729224	-0.260470
C	1.062631	0.613164	-0.130497
C	2.394826	0.909962	0.125285
C	3.333001	-0.103414	0.227220
C	2.960822	-1.428593	0.071616
C	1.635628	-1.737372	-0.171717
H	2.706429	1.932478	0.275299
H	4.362581	0.146083	0.432940
H	3.697181	-2.212784	0.148560
H	1.304752	-2.757797	-0.289505
C	-0.721635	-1.074219	-0.477792
C	-1.783625	0.003867	-0.234733
C	-1.243893	1.383150	-0.408443
C	0.051586	1.660117	-0.304371
H	-1.960634	2.175918	-0.558398
O	-1.085612	-2.176131	-0.807731
O	0.470428	2.950496	-0.327434
H	1.304929	3.017503	-0.788642
O	-2.811023	-0.162636	-1.149668
N	-2.328958	-0.232427	1.092503
H	-3.033375	-1.097925	-1.130431
H	-3.076659	0.431304	1.228318
C	-1.399005	-0.205723	2.197283
H	-1.961240	-0.247272	3.124646
H	-0.757741	0.681056	2.221627
H	-0.759793	-1.085714	2.166445

P-H4-13

C	0.886199	-0.742602	-0.133568
C	1.141765	0.632455	-0.093998
C	2.420454	1.059911	0.235576
C	3.419777	0.138518	0.504348
C	3.163613	-1.220882	0.440309
C	1.892315	-1.659044	0.116142
H	2.639048	2.114327	0.311351
H	4.406134	0.488175	0.767771
H	3.947511	-1.931889	0.647783
H	1.653839	-2.709889	0.057015
C	-0.471495	-1.206004	-0.461441
C	-1.615002	-0.220665	-0.230882
C	-1.198686	1.181653	-0.551112
C	0.067224	1.569713	-0.440468
H	-1.964686	1.889337	-0.824805
O	-0.716645	-2.322783	-0.842799
O	0.396015	2.875138	-0.605797
H	1.251245	2.948332	-1.026546
O	-2.678375	-0.546695	-1.053471
N	-1.997971	-0.425964	1.159302
H	-2.733771	-1.506762	-1.054707
H	-1.186461	-0.353290	1.754881
C	-3.044782	0.461713	1.621153
H	-3.353193	0.151196	2.614958
H	-3.898502	0.364311	0.958067
H	-2.751624	1.514019	1.659304

P-H4-14

C	0.676669	-0.733957	-0.258940
C	1.067113	0.603995	-0.138384
C	2.402284	0.882527	0.118369
C	3.324880	-0.144937	0.230252
C	2.934342	-1.465484	0.083295
C	1.605341	-1.756231	-0.162482
H	2.728562	1.901258	0.262100
H	4.357481	0.090796	0.437107
H	3.659182	-2.259577	0.167331
H	1.260197	-2.772280	-0.276890
C	-0.736959	-1.048114	-0.495577
C	-1.782824	0.037803	-0.225736
C	-1.232398	1.413201	-0.372977
C	0.069168	1.666378	-0.310267
H	-1.947785	2.211293	-0.486874
O	-1.119904	-2.147599	-0.831513
O	0.512220	2.947615	-0.348619
H	1.339430	2.996637	-0.824908
O	-2.814953	-0.137486	-1.136948
N	-2.328250	-0.133701	1.110950
H	-2.826097	-1.071711	-1.366422
H	-2.907598	-0.959584	1.103240
C	-1.406509	-0.143166	2.223122
H	-1.977470	-0.147642	3.146880
H	-0.815424	0.768764	2.210320
H	-0.718278	-0.994388	2.244048

P-H4-15

C	-0.700352	-0.706123	0.247269
C	-1.276255	0.540087	-0.012155
C	-2.628312	0.602310	-0.320716
C	-3.394896	-0.550842	-0.347440
C	-2.823925	-1.780133	-0.065152
C	-1.475167	-1.852744	0.231854
H	-3.090389	1.545540	-0.570885
H	-4.443448	-0.486169	-0.594083
H	-3.425066	-2.675461	-0.084423
H	-0.993906	-2.792541	0.454515
C	0.742341	-0.818318	0.559863
C	1.633407	0.374906	0.207207
C	0.882761	1.667504	0.187405
C	-0.438229	1.738752	0.071700
H	1.466214	2.573180	0.246878
O	1.219763	-1.847502	0.964268
O	-1.041897	2.947913	-0.016172
H	-1.909332	2.913161	0.383380
O	2.652170	0.397220	1.155093
N	2.216740	0.172058	-1.102905
H	3.359182	0.924315	0.781000
H	1.586441	0.461098	-1.831583
C	2.845725	-1.105925	-1.362665
H	3.487972	-1.006811	-2.233247
H	2.144322	-1.925263	-1.532297
H	3.457954	-1.373339	-0.507448

P-H4-16

C	0.723845	-0.713362	-0.235297
C	1.281483	0.541250	0.017735
C	2.628956	0.625242	0.338865
C	3.410493	-0.517102	0.385884
C	2.857708	-1.755339	0.108153
C	1.513271	-1.848467	-0.203597
H	3.077107	1.576239	0.586076
H	4.455018	-0.436881	0.644514
H	3.469397	-2.643054	0.143240
H	1.047898	-2.797062	-0.422100
C	-0.714560	-0.849144	-0.560299
C	-1.618621	0.327962	-0.193818
C	-0.888803	1.632790	-0.216575
C	0.429917	1.726508	-0.094065
H	-1.477113	2.534302	-0.313380
O	-1.168586	-1.873151	-1.000244
O	1.013744	2.945348	-0.043632
H	1.903322	2.899473	-0.389512
O	-2.661658	0.326308	-1.128519
N	-2.029549	0.048448	1.156991
H	-3.221477	1.084168	-0.966517
H	-2.231344	0.893465	1.663467
C	-3.029983	-0.978888	1.342124
H	-3.176195	-1.128195	2.407773
H	-2.680455	-1.912725	0.913130
H	-3.989554	-0.745614	0.878866

P-P1-1

C	0.144815	-0.539438	-0.254114
C	0.998594	0.538627	-0.063045
C	2.363665	0.331779	0.098983
C	2.879416	-0.946144	0.073717
C	2.026130	-2.027231	-0.102182
C	0.668968	-1.823278	-0.258997
H	2.993276	1.195705	0.244841
H	3.939164	-1.106882	0.196168
H	2.421608	-3.031414	-0.111987
H	0.005339	-2.668963	-0.366306
C	-1.346341	-0.358350	-0.428976
C	-1.756081	1.079153	-0.503586
C	-0.952239	2.107967	-0.265425
C	0.480072	1.924023	-0.014378
H	-1.303424	3.128249	-0.278787
H	-2.803000	1.228945	-0.732175
O	1.206250	2.869006	0.208334
O	-1.808667	-0.929796	-1.621485
N	-2.027184	-1.045496	0.652996
H	-1.779579	-1.880916	-1.507546
H	-3.020555	-0.927006	0.517606
C	-1.643570	-0.676651	1.999102
H	-2.301909	-1.183780	2.697274
H	-1.693003	0.398537	2.193623
H	-0.628851	-1.010422	2.194927

P-P1-2

C	0.207978	-0.568437	-0.254656
C	0.968760	0.574683	-0.043378
C	2.336676	0.474921	0.185736
C	2.948886	-0.759561	0.195825
C	2.193691	-1.902241	-0.034415
C	0.833488	-1.806588	-0.254914
H	2.892633	1.386011	0.343528
H	4.010733	-0.837700	0.369879
H	2.671106	-2.870184	-0.047608
H	0.248746	-2.691966	-0.455373
C	-1.294219	-0.506383	-0.405733
C	-1.798081	0.887903	-0.627369
C	-1.061106	1.982522	-0.496625
C	0.355157	1.918390	-0.116554
H	-1.465890	2.971234	-0.648994
H	-2.847825	0.950199	-0.882207
O	0.990865	2.927072	0.102453
O	-1.627460	-1.320600	-1.496683
N	-1.999182	-1.054718	0.741825
H	-2.568997	-1.490277	-1.431455
H	-1.696852	-2.013656	0.839660
C	-1.820800	-0.354972	1.996961
H	-2.316585	-0.919308	2.780321
H	-2.289870	0.622958	1.946098
H	-0.772754	-0.217476	2.277943

P-P1-3

C	0.161397	-0.545327	-0.234945
C	1.000039	0.544241	-0.039231
C	2.365646	0.349976	0.136638
C	2.890329	-0.924719	0.116434
C	2.050341	-2.014423	-0.077003
C	0.692518	-1.825985	-0.248371
H	2.987960	1.218366	0.287255
H	3.950064	-1.076042	0.251603
H	2.458943	-3.013382	-0.090848
H	0.021711	-2.659171	-0.390786
C	-1.329269	-0.393687	-0.419861
C	-1.761416	1.041406	-0.501248
C	-0.968760	2.086074	-0.286820
C	0.464910	1.923436	-0.018261
H	-1.331742	3.102249	-0.315427
H	-2.814425	1.175924	-0.714680
O	1.175318	2.882795	0.193872
O	-1.765092	-1.060829	-1.581744
N	-2.013276	-1.090278	0.640085
H	-1.354935	-0.654194	-2.344103
H	-2.999610	-1.101217	0.430433
C	-1.747834	-0.631354	1.982800
H	-2.357099	-1.208535	2.670995
H	-1.951411	0.431154	2.147029
H	-0.705741	-0.816773	2.230106

P-P1-4

C	0.224285	-0.549500	-0.123012
C	1.220575	0.407031	0.028887
C	2.547166	0.020707	0.176734
C	2.886288	-1.315503	0.175129
C	1.892895	-2.274465	0.035472
C	0.572489	-1.892715	-0.107316
H	3.289429	0.795119	0.292536
H	3.916790	-1.614682	0.286709
H	2.149171	-3.322874	0.041644
H	-0.200161	-2.642843	-0.191056
C	-1.231919	-0.175624	-0.292988
C	-1.452473	1.307062	-0.333999
C	-0.505960	2.219142	-0.153072
C	0.896990	1.850691	0.049678
H	-0.718654	3.276939	-0.170884
H	-2.472619	1.605642	-0.527858
O	1.752218	2.693381	0.218495
O	-1.744217	-0.629605	-1.520436
N	-1.966073	-0.835542	0.767103
H	-1.775751	-1.586321	-1.476921
H	-1.459609	-0.780352	1.635202
C	-3.356005	-0.466811	0.925053
H	-3.843819	-1.197831	1.563113
H	-3.839877	-0.498602	-0.047121
H	-3.512379	0.524294	1.357043

P-P1-5

C	-0.013068	0.449935	0.270932
C	1.167424	-0.213284	-0.052208
C	2.352845	0.493977	-0.203985
C	2.372822	1.861062	-0.020564
C	1.205414	2.520125	0.334904
C	0.020937	1.820189	0.479239
H	3.246375	-0.059489	-0.447934
H	3.294180	2.410850	-0.133620
H	1.219050	3.585714	0.506407
H	-0.883420	2.327396	0.775113
C	-1.326882	-0.295450	0.323824
C	-1.134532	-1.770764	0.529494
C	0.002248	-2.408957	0.285417
C	1.209056	-1.688827	-0.141767
H	0.095521	-3.479819	0.380345
H	-2.025395	-2.307347	0.826064
O	2.199333	-2.285675	-0.505682
O	-2.071069	0.261168	1.371469
N	-2.122348	-0.190753	-0.889197
H	-2.975017	-0.033333	1.249244
H	-1.752376	-0.801215	-1.599262
C	-2.362437	1.137005	-1.410178
H	-3.094241	1.065155	-2.209381
H	-1.469623	1.635289	-1.792987
H	-2.787692	1.758062	-0.626566

P-P1-6

C	0.230624	-0.549391	-0.130444
C	1.205644	0.419879	0.067489
C	2.533964	0.050935	0.238481
C	2.894511	-1.279923	0.207495
C	1.925242	-2.248782	-0.010532
C	0.602280	-1.884935	-0.180852
H	3.261965	0.833084	0.388310
H	3.926234	-1.565820	0.340478
H	2.203592	-3.290709	-0.053630
H	-0.150719	-2.634753	-0.375275
C	-1.232879	-0.196026	-0.258739
C	-1.460623	1.275440	-0.448395
C	-0.520754	2.201335	-0.306523
C	0.861480	1.857783	0.043569
H	-0.728032	3.252687	-0.433898
H	-2.471487	1.551471	-0.712637
O	1.686339	2.717660	0.266000
O	-1.802599	-0.885858	-1.366657
N	-1.892865	-0.621637	0.934449
H	-1.340569	-0.639705	-2.167635
H	-1.622430	-1.569282	1.140515
C	-3.332826	-0.472252	0.967001
H	-3.707315	-0.982187	1.848881
H	-3.832130	-0.878472	0.086560
H	-3.598955	0.576352	1.071150

P-P1-7

C	0.153252	-0.542299	-0.253980
C	0.984923	0.548922	-0.034545
C	2.349625	0.364676	0.157274
C	2.888481	-0.903758	0.128348
C	2.061504	-1.996468	-0.097229
C	0.704466	-1.815729	-0.283625
H	2.961261	1.238066	0.322601
H	3.947478	-1.047229	0.276074
H	2.478715	-2.991490	-0.127108
H	0.060660	-2.664693	-0.462984
C	-1.348330	-0.391597	-0.407046
C	-1.780742	1.039648	-0.515007
C	-0.981713	2.085369	-0.339315
C	0.445044	1.927443	-0.035830
H	-1.340125	3.101215	-0.406660
H	-2.834087	1.154978	-0.726343
O	1.150854	2.888187	0.183913
O	-1.787672	-1.099546	-1.541880
N	-2.097740	-0.991680	0.670190
H	-1.238151	-0.859898	-2.286636
H	-2.079064	-1.991509	0.539609
C	-1.699047	-0.614766	2.004771
H	-2.361701	-1.098827	2.715265
H	-1.814437	0.459236	2.130543
H	-0.666593	-0.875854	2.255147

P-P1-8

C	-0.220265	-0.548091	0.112579
C	-1.225798	0.397492	-0.048483
C	-2.547453	-0.008206	-0.194973
C	-2.865227	-1.349576	-0.177895
C	-1.860607	-2.294706	-0.013148
C	-0.545324	-1.896600	0.129106
H	-3.301948	0.752954	-0.319010
H	-3.891108	-1.664468	-0.290221
H	-2.106886	-3.345480	0.003157
H	0.249333	-2.615183	0.255745
C	1.232440	-0.166830	0.267128
C	1.438139	1.320119	0.330964
C	0.479346	2.226398	0.171577
C	-0.918155	1.844360	-0.054900
H	0.678937	3.286709	0.203990
H	2.458392	1.628429	0.513076
O	-1.778367	2.681640	-0.226134
O	1.776899	-0.735879	1.440226
N	1.964924	-0.784058	-0.807691
H	1.337632	-0.355881	2.200023
H	1.488371	-0.635664	-1.680843
C	3.377756	-0.491998	-0.891718
H	3.833856	-1.185789	-1.591741
H	3.825961	-0.661968	0.082078
H	3.615636	0.524491	-1.216566

P-P1-9

C	-0.029217	-0.444424	-0.206004
C	1.189719	0.163680	0.077793
C	2.343756	-0.598549	0.196725
C	2.295381	-1.966015	0.019124
C	1.089697	-2.571826	-0.299330
C	-0.063489	-1.815742	-0.413197
H	3.268399	-0.087006	0.414693
H	3.193050	-2.557542	0.109898
H	1.047031	-3.637906	-0.462486
H	-1.000218	-2.285610	-0.670814
C	-1.306184	0.364391	-0.280267
C	-1.042556	1.832800	-0.450968
C	0.129122	2.414405	-0.234687
C	1.307114	1.636430	0.162521
H	0.268378	3.480927	-0.320020
H	-1.913544	2.412382	-0.728151
O	2.338203	2.179594	0.494939
O	-2.106653	-0.089296	-1.363017
N	-2.059290	0.244400	0.930460
H	-1.577671	-0.123117	-2.159759
H	-2.818384	0.905766	0.901592
C	-2.554578	-1.068348	1.284702
H	-3.256326	-0.951691	2.104657
H	-1.740017	-1.692104	1.640710
H	-3.060655	-1.578091	0.462604

P-P1-10

C	-0.034533	-0.440924	-0.231890
C	1.195841	0.142533	0.061778
C	2.332034	-0.642869	0.201996
C	2.255727	-2.010996	0.038680
C	1.039617	-2.594314	-0.282988
C	-0.096219	-1.815569	-0.418158
H	3.265669	-0.149289	0.423375
H	3.139306	-2.620815	0.144789
H	0.975556	-3.661474	-0.431755
H	-1.040240	-2.270267	-0.676662
C	-1.301078	0.391595	-0.295013
C	-1.016830	1.856428	-0.450793
C	0.165869	2.415128	-0.224590
C	1.338540	1.613674	0.145140
H	0.321850	3.480987	-0.290602
H	-1.888631	2.442204	-0.703447
O	2.383053	2.138488	0.465856
O	-2.119681	-0.051893	-1.348784
N	-2.125937	0.297405	0.886915
H	-1.580679	-0.158718	-2.131075
H	-1.667804	0.757324	1.655637
C	-2.617415	-1.008402	1.257184
H	-3.350091	-0.884188	2.049297
H	-1.845803	-1.700597	1.604098
H	-3.123871	-1.447461	0.403298

P-P2-1

C	-1.051149	0.596076	-0.049529
C	-0.670132	-0.745085	-0.146501
C	-1.615342	-1.751837	-0.019917
C	-2.944351	-1.435249	0.179658
C	-3.324695	-0.104235	0.273003
C	-2.387539	0.906759	0.165977
H	-1.279527	-2.775180	-0.085221
H	-3.682204	-2.217633	0.264415
H	-4.361657	0.147925	0.434352
H	-2.679685	1.940408	0.249539
C	-0.038848	1.643259	-0.151685
C	1.235699	1.376490	-0.426644
C	1.723679	0.000329	-0.722061
C	0.747350	-1.100692	-0.330173
O	-0.532075	2.885319	0.055452
H	1.968075	2.168315	-0.507951
O	1.145084	-2.237743	-0.216220
H	1.785613	-0.095406	-1.813948
H	0.165513	3.531327	-0.036435
N	3.057174	-0.211468	-0.216111
H	3.377491	-1.106627	-0.550511
C	3.138512	-0.186061	1.228763
H	4.167913	-0.358210	1.528615
H	2.507029	-0.931588	1.720636
H	2.848041	0.797805	1.590088

P-P2-2

C	-1.124222	0.614750	-0.021242
C	-0.790499	-0.742323	-0.022542
C	-1.784106	-1.708775	-0.046420
C	-3.112394	-1.335698	-0.098782
C	-3.446047	0.011039	-0.102645
C	-2.462888	0.982247	-0.056192
H	-1.487222	-2.745843	-0.025813
H	-3.886286	-2.086389	-0.132547
H	-4.483405	0.307124	-0.136240
H	-2.720650	2.028323	-0.041190
C	-0.062541	1.613116	0.059568
C	1.223280	1.281099	-0.015489
C	1.667738	-0.121682	-0.267347
C	0.618501	-1.157570	0.061144
O	-0.524854	2.873896	0.223948
H	1.993856	2.035531	0.058101
O	0.943511	-2.292767	0.324096
H	1.766732	-0.234811	-1.367219
H	0.207132	3.485640	0.270153
N	2.901132	-0.449361	0.390272
H	2.923496	-1.449221	0.522279
C	4.076423	0.014849	-0.298132
H	4.962104	-0.339668	0.220524
H	4.116320	1.102787	-0.291922
H	4.131275	-0.313294	-1.343913

P-P2-3

C	1.211203	0.526016	0.034494
C	0.637755	-0.747516	-0.004288
C	1.440186	-1.877283	0.014199
C	2.812508	-1.750998	0.110533
C	3.383326	-0.487532	0.154544
C	2.592663	0.646087	0.106008
H	0.963714	-2.843646	-0.045410
H	3.437020	-2.629914	0.145760
H	4.455736	-0.384968	0.220035
H	3.034853	1.628648	0.118016
C	0.346337	1.699284	-0.047846
C	-0.979705	1.601710	0.018664
C	-1.672422	0.300055	0.268524
C	-0.824726	-0.889217	-0.149281
O	1.026123	2.859401	-0.192307
H	-1.618059	2.471878	-0.035141
O	-1.329715	-1.904952	-0.565659
H	-1.759509	0.187385	1.358830
H	0.414498	3.592705	-0.217742
N	-3.010312	0.292632	-0.257851
H	-2.981901	0.049238	-1.235691
C	-3.927558	-0.583055	0.439652
H	-4.902225	-0.522905	-0.036550
H	-4.046151	-0.229955	1.462765
H	-3.614455	-1.627797	0.462585

P-P2-4

C	-1.061879	0.596539	-0.050146
C	-0.671118	-0.746436	-0.098785
C	-1.609741	-1.758015	0.025145
C	-2.949666	-1.453006	0.167884
C	-3.346764	-0.125471	0.190700
C	-2.413725	0.890686	0.085075
H	-1.260901	-2.778865	-0.002174
H	-3.681715	-2.240747	0.250838
H	-4.392736	0.122371	0.286649
H	-2.752115	1.915688	0.077826
C	-0.043870	1.645252	-0.115732
C	1.226573	1.375263	-0.397286
C	1.699455	0.001927	-0.727980
C	0.752441	-1.094582	-0.263860
O	-0.436746	2.931928	0.066514
H	1.948485	2.175429	-0.451080
O	1.160980	-2.220617	-0.097553
H	1.678308	-0.094283	-1.822313
H	-1.121697	2.975192	0.731401
N	3.064507	-0.203980	-0.318712
H	3.360111	-1.106062	-0.656652
C	3.254419	-0.146212	1.115072
H	4.301699	-0.324036	1.340262
H	2.654221	-0.872648	1.670453
H	3.004168	0.849664	1.473560

P-P2-5

C	-1.120864	0.518749	-0.017327
C	-0.541198	-0.736406	-0.205965
C	-1.301085	-1.884758	-0.062800
C	-2.635349	-1.794167	0.286208
C	-3.212608	-0.547925	0.474138
C	-2.464279	0.605513	0.317600
H	-0.822648	-2.837091	-0.230715
H	-3.225785	-2.688897	0.407582
H	-4.255771	-0.472832	0.740493
H	-2.913256	1.575886	0.450990
C	-0.304264	1.716868	-0.202258
C	1.009096	1.660267	-0.417454
C	1.758739	0.374028	-0.411947
C	0.875808	-0.842523	-0.606026
O	-1.016710	2.861275	-0.142158
H	1.579552	2.569990	-0.553637
O	1.346269	-1.876796	-1.018543
H	2.492235	0.365215	-1.226757
H	-0.437176	3.613486	-0.246575
N	2.405251	0.172779	0.878111
H	2.594823	1.061914	1.307680
C	3.578968	-0.665393	0.840955
H	3.999844	-0.732404	1.839985
H	4.352245	-0.299173	0.155540
H	3.304922	-1.666900	0.523502

P-P2-6

C	1.118837	0.622650	0.016096
C	0.787871	-0.736912	0.056810
C	1.778415	-1.705851	0.073054
C	3.110435	-1.342365	0.075294
C	3.447133	0.000925	0.022000
C	2.463691	0.972614	-0.019566
H	1.473899	-2.740939	0.080913
H	3.881573	-2.095755	0.104294
H	4.484928	0.296111	-0.000217
H	2.762106	2.006084	-0.107886
C	0.049130	1.619822	-0.023337
C	-1.232099	1.277736	0.055807
C	-1.680006	-0.125874	0.275306
C	-0.620583	-1.161334	-0.009051
O	0.384190	2.923500	-0.209071
H	-1.982220	2.051755	0.017170
O	-0.933920	-2.306899	-0.239389
H	-1.818084	-0.233384	1.372402
H	1.178193	3.136821	0.276270
N	-2.888430	-0.460409	-0.424703
H	-2.918910	-1.463768	-0.522692
C	-4.087171	0.041506	0.193953
H	-4.952675	-0.327492	-0.347975
H	-4.116412	1.127975	0.141621
H	-4.189474	-0.244843	1.248509

P-P2-7

C	-1.080907	0.598026	-0.033886
C	-0.687229	-0.739263	-0.119358
C	-1.632625	-1.749369	-0.034249
C	-2.971276	-1.438789	0.105250
C	-3.363054	-0.110740	0.188015
C	-2.425821	0.903905	0.128026
H	-1.290151	-2.771426	-0.082144
H	-3.707791	-2.225561	0.153916
H	-4.407220	0.135620	0.305711
H	-2.723673	1.936312	0.208811
C	-0.064430	1.643156	-0.082325
C	1.209276	1.367093	-0.352823
C	1.686126	-0.011758	-0.714023
C	0.743143	-1.101434	-0.232373
O	-0.550922	2.880241	0.164854
H	1.944378	2.161059	-0.395678
O	1.127804	-2.218643	0.004306
H	1.614124	-0.103923	-1.806285
H	0.151127	3.525019	0.104748
N	3.047937	-0.306657	-0.368265
H	3.671894	0.277949	-0.897243
C	3.340021	-0.247685	1.043136
H	4.402116	-0.416196	1.193447
H	2.806944	-1.046871	1.550752
H	3.068289	0.702973	1.516212

P-P2-8

C	-1.111930	0.505942	-0.021598
C	-0.490767	-0.724367	-0.257124
C	-1.198837	-1.906537	-0.128937
C	-2.527393	-1.885412	0.254383
C	-3.143123	-0.671611	0.510228
C	-2.443237	0.515508	0.374239
H	-0.683491	-2.831816	-0.336151
H	-3.078561	-2.806646	0.358959
H	-4.175670	-0.645913	0.822970
H	-2.938047	1.445873	0.609060
C	-0.344029	1.741138	-0.206304
C	0.971180	1.735675	-0.402719
C	1.765523	0.477598	-0.410897
C	0.929838	-0.759901	-0.666114
O	-1.005759	2.920804	-0.111304
H	1.497352	2.672382	-0.495503
O	1.437318	-1.767171	-1.104608
H	2.514860	0.510639	-1.202100
H	-1.888572	2.832980	-0.466104
N	2.484425	0.356235	0.847434
H	1.840582	0.378044	1.622283
C	3.423120	-0.735886	0.948294
H	3.949054	-0.652451	1.895448
H	4.155810	-0.646489	0.149447
H	2.981160	-1.732187	0.876242

P-P2-9

C	-1.014919	0.633713	-0.055590
C	-0.764082	-0.736818	-0.148232
C	-1.781854	-1.650109	0.075519
C	-3.048909	-1.209552	0.406028
C	-3.300249	0.151317	0.495736
C	-2.293758	1.071003	0.261471
H	-1.552379	-2.700251	-0.017944
H	-3.839774	-1.920237	0.588385
H	-4.290440	0.499748	0.746630
H	-2.489468	2.128961	0.319334
C	0.069747	1.578698	-0.312814
C	1.326840	1.186462	-0.517150
C	1.742242	-0.247315	-0.419191
C	0.579673	-1.221975	-0.522129
O	-0.338341	2.867106	-0.314287
H	2.098725	1.923401	-0.695441
O	0.766723	-2.360074	-0.872745
H	2.403260	-0.505994	-1.245587
H	0.406798	3.444353	-0.469342
N	2.470771	-0.560901	0.802010
H	1.952468	-0.217892	1.595990
C	3.819848	-0.050981	0.827525
H	4.284683	-0.321103	1.771389
H	3.902313	1.035270	0.708550
H	4.393889	-0.522871	0.033186

P-P2-10

C	-1.101388	0.519629	-0.012494
C	-0.519446	-0.727528	-0.252989
C	-1.261512	-1.886713	-0.118840
C	-2.584728	-1.825112	0.279522
C	-3.161401	-0.594285	0.542134
C	-2.427146	0.570924	0.395957
H	-0.776692	-2.827730	-0.328041
H	-3.161074	-2.729801	0.392719
H	-4.188694	-0.537657	0.867627
H	-2.892727	1.515386	0.635764
C	-0.301599	1.729419	-0.223786
C	1.011311	1.681239	-0.431034
C	1.768131	0.400189	-0.397805
C	0.898147	-0.809790	-0.665053
O	-0.929505	2.927135	-0.174482
H	1.553180	2.601783	-0.586572
O	1.369071	-1.823201	-1.124419
H	2.547120	0.409617	-1.168334
H	-1.836430	2.836931	-0.461095
N	2.334687	0.173829	0.924804
H	2.500392	1.054698	1.380835
C	3.506282	-0.667954	0.939502
H	3.863232	-0.764171	1.960740
H	4.322244	-0.287485	0.314423
H	3.250194	-1.659955	0.578838

P-P2-11

C	-1.088098	0.598283	-0.036947
C	-0.683988	-0.740030	-0.077126
C	-1.620461	-1.756885	0.005055
C	-2.967791	-1.460295	0.091169
C	-3.375967	-0.136370	0.106819
C	-2.445240	0.885723	0.047929
H	-1.265169	-2.775770	-0.007077
H	-3.696745	-2.253893	0.138513
H	-4.426668	0.103569	0.162075
H	-2.786937	1.909911	0.038938
C	-0.068546	1.645870	-0.048691
C	1.202315	1.368291	-0.320424
C	1.665546	-0.005681	-0.713806
C	0.752597	-1.090276	-0.173744
O	-0.455078	2.926490	0.178149
H	1.928080	2.168301	-0.326821
O	1.149676	-2.191415	0.110552
H	1.524930	-0.098220	-1.799865
H	-1.172187	2.945650	0.809622
N	3.046246	-0.293906	-0.450774
H	3.630991	0.293921	-1.019708
C	3.425674	-0.218490	0.939734
H	4.496176	-0.379500	1.023940
H	2.930654	-1.014605	1.488530
H	3.180120	0.736540	1.417846

P-O1-1

C	0.651793	-0.323961	-0.155012
C	1.229957	0.899502	0.183793
C	2.610247	0.984781	0.319992
C	3.406704	-0.126768	0.112738
C	2.826004	-1.331507	-0.243765
C	1.448399	-1.429348	-0.375242
H	3.058299	1.932913	0.579381
H	4.477593	-0.050277	0.218403
H	3.444649	-2.196983	-0.424423
H	0.984821	-2.358655	-0.668231
C	-0.847081	-0.452445	-0.184785
C	-1.536578	0.878887	-0.483179
C	-0.906855	2.089860	0.016369
C	0.395005	2.079127	0.322067
H	-1.501271	2.989016	0.039586
O	-2.594820	0.863627	-1.074174
H	0.880730	2.992817	0.635680
O	-1.232147	-1.388742	-1.140925
N	-1.256911	-0.779341	1.160997
H	-2.059895	-1.071698	-1.516954
H	-0.641230	-1.485846	1.529457
C	-2.643190	-1.159295	1.326571
H	-2.803449	-1.424987	2.366902
H	-2.938053	-2.002580	0.699389
H	-3.294496	-0.320418	1.097349

P-O1-2

C	0.509891	-0.191342	-0.224628
C	1.022591	1.029042	0.216553
C	2.399869	1.204760	0.291971
C	3.259057	0.188999	-0.082285
C	2.743096	-1.007325	-0.550815
C	1.371216	-1.195144	-0.621000
H	2.793421	2.151651	0.631831
H	4.326324	0.334726	-0.022981
H	3.408502	-1.796708	-0.864694
H	0.959207	-2.119345	-0.995339
C	-0.977315	-0.413727	-0.215203
C	-1.780884	0.885061	-0.284645
C	-1.190114	2.089188	0.265572
C	0.125385	2.131253	0.506632
H	-1.834928	2.941143	0.409031
O	-2.909235	0.819997	-0.725448
H	0.571607	3.041284	0.883504
O	-1.324087	-1.231496	-1.291734
N	-1.376955	-0.937829	1.068762
H	-2.236803	-1.016142	-1.507967
H	-2.385323	-0.968157	1.093282
C	-0.825062	-2.225820	1.430095
H	-1.348142	-2.587693	2.309844
H	0.224424	-2.123957	1.690350
H	-0.919401	-2.969686	0.635778

P-O1-3

C	0.667499	-0.341196	-0.147914
C	1.223370	0.901788	0.154609
C	2.602808	1.016960	0.291527
C	3.416571	-0.086576	0.118291
C	2.855437	-1.314336	-0.193563
C	1.481209	-1.442167	-0.319496
H	3.034044	1.980051	0.522885
H	4.486075	0.010650	0.221152
H	3.489290	-2.175957	-0.335817
H	1.027429	-2.391136	-0.556826
C	-0.826560	-0.492504	-0.191453
C	-1.535067	0.817698	-0.527852
C	-0.938151	2.049686	-0.032295
C	0.365641	2.069342	0.270916
H	-1.551047	2.936891	-0.018874
O	-2.598981	0.773912	-1.109477
H	0.833665	2.996561	0.572173
O	-1.209576	-1.455078	-1.106911
N	-1.250220	-0.888121	1.142960
H	-2.010427	-1.126977	-1.529412
H	-0.792332	-0.332278	1.846761
C	-2.671774	-1.012691	1.365153
H	-2.827289	-1.467907	2.338832
H	-3.083899	-1.685377	0.619008
H	-3.231406	-0.074366	1.322963

P-O1-4

C	-0.498194	-0.190368	0.262653
C	-0.997812	1.023803	-0.215306
C	-2.371892	1.216210	-0.293558
C	-3.243001	0.221518	0.112031
C	-2.740987	-0.969216	0.608404
C	-1.370925	-1.175358	0.680462
H	-2.754933	2.158117	-0.658695
H	-4.308457	0.379511	0.052637
H	-3.416646	-1.741501	0.942522
H	-0.969330	-2.096070	1.074054
C	0.987861	-0.431601	0.200425
C	1.790674	0.862320	0.335983
C	1.235127	2.048373	-0.302100
C	-0.079743	2.098950	-0.553269
H	1.890826	2.887572	-0.470790
O	2.853871	0.832930	0.907926
H	-0.510161	2.998907	-0.971108
O	1.356797	-1.318473	1.190048
N	1.401418	-0.949409	-1.100121
H	2.290693	-1.154668	1.358007
H	1.265712	-0.249525	-1.813691
C	0.795604	-2.205721	-1.479822
H	1.291045	-2.572238	-2.374130
H	-0.278921	-2.147698	-1.672363
H	0.964619	-2.925664	-0.684807

P-O1-5

C	0.572200	-0.357009	-0.214596
C	0.995562	0.963121	-0.061742
C	2.356172	1.239145	0.044222
C	3.285057	0.219665	-0.017791
C	2.859090	-1.087834	-0.193946
C	1.507551	-1.373671	-0.286656
H	2.679722	2.262968	0.163284
H	4.337813	0.442100	0.059380
H	3.581996	-1.885950	-0.264219
H	1.168064	-2.387224	-0.437584
C	-0.899390	-0.682240	-0.197093
C	-1.791288	0.513809	-0.552861
C	-1.281015	1.853707	-0.319787
C	0.023019	2.040918	-0.080819
H	-1.978564	2.672481	-0.398407
O	-2.897099	0.282950	-0.984284
H	0.401431	3.044071	0.061475
O	-1.134009	-1.708214	-1.095820
N	-1.333308	-1.137399	1.115437
H	-2.090397	-1.755759	-1.190677
H	-0.802584	-1.969309	1.326576
C	-1.273524	-0.196640	2.209895
H	-1.498056	-0.727407	3.129635
H	-2.033608	0.570741	2.083329
H	-0.304401	0.299373	2.327028

P-O1-6

C	0.544315	-0.252757	-0.151563
C	1.103722	0.998281	0.110696
C	2.480455	1.111331	0.265981
C	3.295084	-0.001522	0.168023
C	2.734543	-1.241855	-0.083390
C	1.363030	-1.363128	-0.245346
H	2.910354	2.081375	0.468915
H	4.362128	0.097961	0.292194
H	3.362959	-2.116442	-0.151538
H	0.910761	-2.325588	-0.435237
C	-0.931165	-0.371255	-0.457302
C	-1.758050	0.828005	0.049663
C	-1.084067	2.107565	0.214405
C	0.250555	2.166014	0.246226
H	-1.704950	2.975918	0.367801
O	-2.937668	0.674819	0.258452
H	0.742941	3.114475	0.411742
O	-1.123854	-0.270909	-1.847273
N	-1.461634	-1.627052	-0.022925
H	-0.659966	-1.006699	-2.249791
H	-2.420627	-1.646367	-0.339813
C	-1.424092	-1.851782	1.408145
H	-1.883968	-2.811591	1.621898
H	-1.949007	-1.084628	1.982588
H	-0.392995	-1.893705	1.749053

P-O1-7

C	0.668673	-0.326006	-0.159150
C	1.220806	0.919688	0.142118
C	2.597174	1.040957	0.298978
C	3.421106	-0.058622	0.151453
C	2.870385	-1.289778	-0.160694
C	1.499066	-1.418816	-0.312444
H	3.018570	2.009045	0.527418
H	4.488159	0.045134	0.271634
H	3.507485	-2.151298	-0.287597
H	1.072013	-2.376652	-0.563792
C	-0.831945	-0.501475	-0.232216
C	-1.571699	0.811468	-0.526378
C	-0.938300	2.049473	-0.072361
C	0.361179	2.086116	0.234564
H	-1.557396	2.932779	-0.067766
O	-2.681038	0.801078	-0.999238
H	0.823889	3.020176	0.522488
O	-1.212189	-1.424055	-1.197569
N	-1.258746	-0.987856	1.066926
H	-1.254502	-2.273071	-0.757477
H	-0.695865	-0.603179	1.806647
C	-2.677369	-0.950099	1.361843
H	-2.867562	-1.589833	2.218745
H	-3.226019	-1.339777	0.509989
H	-3.066181	0.048047	1.571411

P-O1-8

C	0.532797	-0.258430	-0.143899
C	1.132299	0.979613	0.106587
C	2.508161	1.052797	0.289087
C	3.287911	-0.087905	0.235560
C	2.692284	-1.313875	-0.001862
C	1.321550	-1.392381	-0.193816
H	2.964321	2.013003	0.481259
H	4.354435	-0.020655	0.383263
H	3.291923	-2.210106	-0.038060
H	0.861109	-2.350858	-0.381334
C	-0.953240	-0.329430	-0.473048
C	-1.729000	0.849628	0.150943
C	-1.023802	2.134485	0.204034
C	0.310102	2.176311	0.202644
H	-1.629536	3.016244	0.341206
O	-2.870721	0.740893	0.514068
H	0.824211	3.120551	0.318495
O	-1.100508	-0.157318	-1.870563
N	-1.603510	-1.554241	-0.180782
H	-0.353864	0.337931	-2.204666
H	-1.327383	-2.257263	-0.843810
C	-1.599168	-1.993408	1.189089
H	-2.127716	-2.939402	1.253052
H	-2.142901	-1.276903	1.797874
H	-0.599575	-2.125872	1.618233

P-O2-1

C	-1.030915	0.534679	-0.051845
C	-0.856672	-0.906718	-0.229309
C	-2.034771	-1.735287	-0.128349
C	-3.244313	-1.205796	0.114815
C	-3.402320	0.213704	0.282669
C	-2.346868	1.045128	0.205646
H	-1.911007	-2.799911	-0.258883
H	-4.112676	-1.842069	0.184748
H	-4.387208	0.610012	0.475987
H	-2.458421	2.109399	0.335670
C	0.048153	1.364244	-0.088070
C	1.388146	0.854579	-0.268952
C	1.552233	-0.587567	-0.684223
C	0.359855	-1.436529	-0.464883
O	-0.046372	2.674282	0.158454
O	2.344075	1.607205	-0.152354
H	0.493098	-2.500884	-0.591455
H	1.596577	-0.485277	-1.782193
H	0.857146	3.014359	0.131513
N	2.779968	-1.201351	-0.260756
H	3.546998	-0.639769	-0.595369
C	2.873438	-1.331704	1.178988
H	3.815877	-1.807038	1.433082
H	2.071036	-1.975249	1.533304
H	2.811383	-0.378415	1.711168

P-O2-2

C	-1.155281	0.457009	-0.068151
C	-0.779252	-0.952871	0.004373
C	-1.845385	-1.921518	0.089448
C	-3.134545	-1.545417	0.085989
C	-3.490919	-0.155691	-0.002983
C	-2.547368	0.801789	-0.074874
H	-1.571997	-2.964259	0.151399
H	-3.917315	-2.285176	0.147540
H	-4.535234	0.116010	-0.007677
H	-2.808789	1.845896	-0.133319
C	-0.193349	1.421170	-0.074080
C	1.209209	1.093321	0.010142
C	1.600327	-0.337888	-0.196909
C	0.517058	-1.322796	0.016084
O	-0.486338	2.724600	-0.036696
O	2.037831	1.980205	0.157723
H	0.789893	-2.364423	0.093645
H	1.700886	-0.330699	-1.311068
H	0.359163	3.187062	0.020624
N	2.848604	-0.628484	0.438185
H	3.371211	0.232467	0.496203
C	3.615971	-1.669292	-0.195272
H	4.574698	-1.762506	0.305265
H	3.796594	-1.492882	-1.262876
H	3.109928	-2.627444	-0.097849

P-O2-3

C	-1.140373	0.487255	-0.076488
C	-0.947655	-0.959619	-0.006515
C	-2.129144	-1.785704	0.063610
C	-3.359652	-1.248246	0.053389
C	-3.535725	0.176742	-0.025542
C	-2.477886	1.006800	-0.084746
H	-1.990535	-2.855061	0.118548
H	-4.230876	-1.882593	0.102266
H	-4.537027	0.579023	-0.033223
H	-2.603943	2.076126	-0.135955
C	-0.062980	1.319456	-0.070680
C	1.289546	0.813922	0.042251
C	1.502567	-0.661956	-0.188281
C	0.290451	-1.492571	0.006678
O	-0.188525	2.649012	-0.010448
O	2.202952	1.595785	0.258054
H	0.447077	-2.558788	0.067403
H	1.634781	-0.674125	-1.285942
H	0.708940	2.995363	0.075470
N	2.688603	-1.231089	0.384493
H	2.747053	-0.983441	1.358999
C	3.924663	-0.904955	-0.296258
H	4.744670	-1.406706	0.209616
H	4.138535	0.162532	-0.343926
H	3.882808	-1.299822	-1.310063

P-O2-4

C	1.141663	0.491800	0.056908
C	0.943339	-0.954292	0.020900
C	2.123287	-1.783972	-0.034542
C	3.354272	-1.247836	-0.045476
C	3.536152	0.178221	-0.002102
C	2.479715	1.010104	0.044752
H	1.984700	-2.854419	-0.064085
H	4.223362	-1.885869	-0.085615
H	4.538473	0.577515	-0.011210
H	2.606186	2.080338	0.070605
C	0.064204	1.321500	0.055594
C	-1.296705	0.819311	-0.022078
C	-1.507329	-0.652392	0.208480
C	-0.295460	-1.483600	0.029231
O	0.183006	2.648164	-0.011439
O	-2.206078	1.615625	-0.181949
H	-0.428475	-2.556366	0.006838
H	-1.639941	-0.649254	1.317254
H	-0.719670	2.988963	-0.074359
N	-2.671176	-1.168128	-0.450877
H	-2.564601	-2.157037	-0.598819
C	-3.929008	-0.878998	0.199600
H	-4.729752	-1.370184	-0.345007
H	-4.110784	0.189140	0.176647
H	-3.961469	-1.215329	1.243396

P-O2-5

C	-1.056092	0.520759	-0.061975
C	-0.860639	-0.921547	-0.190312
C	-2.028108	-1.762284	-0.067590
C	-3.246143	-1.239686	0.146648
C	-3.426399	0.182987	0.261484
C	-2.381020	1.024298	0.164509
H	-1.890678	-2.829430	-0.158753
H	-4.106377	-1.885194	0.232599
H	-4.418502	0.571656	0.431501
H	-2.506386	2.091029	0.256441
C	0.016257	1.356221	-0.103457
C	1.378452	0.866901	-0.240780
C	1.552957	-0.568467	-0.664755
C	0.368308	-1.432462	-0.400045
O	-0.092391	2.668586	0.110549
O	2.299320	1.647480	-0.084140
H	0.508189	-2.501024	-0.490389
H	1.539559	-0.435173	-1.761579
H	0.812343	3.009823	0.105581
N	2.842649	-1.085773	-0.314247
H	3.010561	-1.950831	-0.799045
C	3.042146	-1.231534	1.108569
H	4.005168	-1.699378	1.287823
H	2.266647	-1.825338	1.605674
H	3.067189	-0.245372	1.564836

P-O2-6

C	-1.035058	0.529502	-0.067701
C	-0.823933	-0.915226	-0.197887
C	-1.971099	-1.780702	-0.059783
C	-3.203739	-1.292851	0.147687
C	-3.414363	0.126769	0.222321
C	-2.386881	0.988719	0.119785
H	-1.802111	-2.844412	-0.136948
H	-4.047848	-1.957020	0.244769
H	-4.417810	0.501531	0.352387
H	-2.596485	2.048017	0.150294
C	0.022282	1.391319	-0.076344
C	1.390907	0.903841	-0.228668
C	1.559065	-0.535248	-0.688932
C	0.402045	-1.416999	-0.433643
O	-0.059388	2.708582	0.151889
O	2.358834	1.612449	-0.068647
H	0.563949	-2.480893	-0.527781
H	1.557859	-0.406353	-1.785003
H	-0.919041	2.944683	0.493662
N	2.815878	-1.127612	-0.326731
H	3.552062	-0.524015	-0.657883
C	2.960448	-1.305286	1.103981
H	3.929590	-1.749001	1.310851
H	2.198329	-1.995515	1.460031
H	2.876744	-0.374997	1.671910

P-O2-7

C	-1.141838	0.455280	-0.093876
C	-0.759003	-0.951033	0.048069
C	-1.812247	-1.927275	0.186684
C	-3.107678	-1.580047	0.134012
C	-3.478196	-0.208811	-0.081993
C	-2.546247	0.755569	-0.190810
H	-1.520239	-2.957553	0.325691
H	-3.880394	-2.325596	0.234608
H	-4.523733	0.043786	-0.167952
H	-2.867082	1.768638	-0.384966
C	-0.196376	1.438235	-0.070630
C	1.221155	1.120563	0.065879
C	1.603210	-0.317719	-0.187843
C	0.538085	-1.308411	0.069250
O	-0.457379	2.752305	-0.058014
O	2.066882	1.958155	0.284504
H	0.825527	-2.340288	0.205683
H	1.661839	-0.289759	-1.303801
H	-1.376222	2.915608	0.143870
N	2.872598	-0.618149	0.395729
H	3.377731	0.250022	0.492467
C	3.639956	-1.604848	-0.317796
H	4.610204	-1.718001	0.156045
H	3.796365	-1.358290	-1.375461
H	3.146869	-2.574218	-0.273883

P-O2-8

C	1.120090	0.484104	0.105305
C	0.919819	-0.959387	-0.046159
C	2.089981	-1.794699	-0.168230
C	3.330240	-1.286866	-0.094624
C	3.521875	0.120142	0.126356
C	2.474550	0.959132	0.221452
H	1.932006	-2.853392	-0.310263
H	4.192295	-1.929047	-0.181523
H	4.525958	0.502164	0.227696
H	2.661898	2.004309	0.420385
C	0.058426	1.339194	0.063449
C	-1.300882	0.834070	-0.139050
C	-1.509242	-0.635873	0.177301
C	-0.320912	-1.481478	-0.071303
O	0.152019	2.675792	0.041081
O	-2.213826	1.541836	-0.494323
H	-0.490493	-2.541328	-0.186004
H	-1.576075	-0.600191	1.280238
H	1.046575	2.953095	-0.145768
N	-2.736446	-1.193671	-0.312023
H	-2.874787	-0.892444	-1.264078
C	-3.903163	-0.854362	0.476664
H	-4.782327	-1.288804	0.009625
H	-4.062437	0.219107	0.588710
H	-3.807720	-1.302660	1.464113

P-O2-9

C	-1.066603	0.512407	-0.083926
C	-0.822197	-0.930377	-0.146214
C	-1.951129	-1.813470	0.026135
C	-3.196303	-1.341943	0.192526
C	-3.441111	0.074860	0.187699
C	-2.431018	0.952637	0.056021
H	-1.759569	-2.876080	0.006966
H	-4.026859	-2.019138	0.314696
H	-4.454855	0.431952	0.282061
H	-2.662942	2.007527	0.028253
C	-0.021834	1.387168	-0.095905
C	1.372140	0.923805	-0.170210
C	1.556936	-0.497385	-0.666086
C	0.420176	-1.403749	-0.351380
O	-0.128348	2.708211	0.084676
O	2.296943	1.653025	0.082653
H	0.601768	-2.469160	-0.391116
H	1.472780	-0.323529	-1.754024
H	-1.005706	2.944099	0.378225
N	2.877462	-0.991245	-0.414352
H	3.042750	-1.822211	-0.956173
C	3.167269	-1.208182	0.983239
H	4.153407	-1.652365	1.077991
H	2.442947	-1.857233	1.489799
H	3.187336	-0.249656	1.493754

P-O3-1

C	1.565403	-0.060036	0.292278
C	0.378866	-1.018866	0.249625
C	-0.964669	-0.475790	0.045110
C	-1.175816	0.897074	0.205742
C	-0.070679	1.768435	0.578232
C	1.183433	1.340242	0.648006
O	2.481478	-0.505842	1.253439
N	2.057631	-0.114166	-1.058197
O	0.619217	-2.203977	0.333808
H	-0.309579	2.794270	0.818355
H	1.986568	1.991088	0.958242
H	2.254423	-1.077703	-1.285027
C	3.196750	0.730993	-1.344037
H	3.575298	0.482507	-2.330510
H	4.005637	0.620523	-0.618815
H	2.887474	1.772402	-1.369134
H	2.438556	-1.466304	1.247936
C	-2.016519	-1.327159	-0.256071
C	-3.289040	-0.818759	-0.428231
C	-3.507461	0.543068	-0.276679
C	-2.463811	1.391666	0.044369
H	-1.811150	-2.381873	-0.355310
H	-4.108057	-1.475415	-0.675896
H	-4.501006	0.944888	-0.404488
H	-2.645889	2.448116	0.173997

P-O3-2

C	1.576013	0.432562	0.205055
C	0.565648	-0.659869	0.541142
C	-0.840639	-0.418970	0.198939
C	-1.275700	0.896732	0.012232
C	-0.332118	1.998754	0.151416
C	0.973895	1.798888	0.278950
O	2.644671	0.359152	1.097094
N	1.926164	0.177898	-1.172893
O	0.966421	-1.693944	1.027571
H	-0.735240	3.000967	0.161885
H	1.670758	2.614425	0.405460
H	2.296550	1.015431	-1.590595
C	2.797675	-0.952408	-1.408434
H	2.991865	-1.019321	-2.474478
H	2.307594	-1.873492	-1.104969
H	3.750569	-0.881640	-0.881082
H	2.679427	-0.548011	1.415754
C	-1.730603	-1.477769	0.133324
C	-3.062302	-1.244190	-0.153807
C	-3.502351	0.056531	-0.346591
C	-2.619891	1.118513	-0.254276
H	-1.357906	-2.475562	0.306441
H	-3.755869	-2.067392	-0.222383
H	-4.542745	0.245330	-0.562908
H	-2.974662	2.129681	-0.387890

P-O3-3

C	-1.591179	0.464190	-0.206104
C	-0.594453	-0.624869	-0.581400
C	0.814308	-0.407731	-0.227439
C	1.257745	0.902554	-0.014630
C	0.319404	2.015537	-0.122941
C	-0.989525	1.829333	-0.252614
O	-2.684994	0.383534	-1.047611
N	-1.997465	0.225115	1.171555
O	-1.008589	-1.655233	-1.067969
H	0.730620	3.014212	-0.097846
H	-1.687774	2.647922	-0.329944
H	-1.245634	0.438036	1.806916
C	-2.629541	-1.042178	1.453305
H	-2.972603	-1.030643	2.483556
H	-1.992553	-1.918536	1.304833
H	-3.503902	-1.146308	0.818044
H	-2.686567	-0.506715	-1.413489
C	1.696779	-1.474463	-0.181059
C	3.030017	-1.255802	0.110860
C	3.478048	0.038215	0.329710
C	2.603263	1.108507	0.259398
H	1.316381	-2.465333	-0.376568
H	3.718631	-2.084362	0.161973
H	4.519662	0.215750	0.549701
H	2.965455	2.114005	0.414067

P-O3-4

C	-1.744070	0.098898	-0.303965
C	-0.617593	-0.939978	-0.346013
C	0.767747	-0.486471	-0.181773
C	1.059263	0.878562	-0.280022
C	-0.001677	1.835175	-0.567976
C	-1.279223	1.475249	-0.648171
O	-2.732859	-0.263285	-1.202495
N	-2.309865	0.051866	1.034311
O	-0.924072	-2.099097	-0.491809
H	0.290157	2.861188	-0.740033
H	-2.057232	2.186754	-0.885306
H	-3.091261	0.689650	1.056494
C	-1.411863	0.274323	2.143487
H	-1.998220	0.340775	3.054358
H	-0.804999	1.181319	2.055506
H	-0.739253	-0.573708	2.251527
H	-2.887852	-1.201950	-1.060268
C	1.773485	-1.414313	0.043907
C	3.080309	-0.995183	0.195298
C	3.379002	0.356978	0.102621
C	2.381174	1.283480	-0.138900
H	1.504616	-2.457996	0.099334
H	3.864044	-1.712669	0.380456
H	4.399484	0.690337	0.214220
H	2.625694	2.331966	-0.222996

P-O3-5

C	-1.741169	0.137638	-0.300139
C	-0.625594	-0.911079	-0.370709
C	0.762190	-0.482898	-0.181580
C	1.070365	0.878952	-0.276827
C	0.019781	1.852148	-0.555005
C	-1.265131	1.519651	-0.599347
O	-2.719771	-0.219969	-1.215745
N	-2.334571	0.133031	1.027654
O	-0.947922	-2.069050	-0.532028
H	0.326886	2.873270	-0.729483
H	-2.042432	2.241084	-0.797829
H	-2.902633	-0.697553	1.101472
C	-1.443978	0.264410	2.158431
H	-2.039979	0.369485	3.060054
H	-0.852208	1.169996	2.050564
H	-0.755988	-0.575106	2.299297
H	-2.673620	-1.176966	-1.306878
C	1.754730	-1.424560	0.044107
C	3.066319	-1.021946	0.201468
C	3.381389	0.326369	0.112430
C	2.396022	1.266679	-0.130638
H	1.473267	-2.465193	0.093640
H	3.840827	-1.749230	0.386996
H	4.405485	0.646889	0.228478
H	2.654384	2.312081	-0.210866

P-O3-6

C	-1.574301	-0.103664	-0.273960
C	-0.383626	-1.062273	-0.287249
C	0.950504	-0.492459	-0.057818
C	1.149019	0.873184	-0.291265
C	0.040942	1.703074	-0.749471
C	-1.208890	1.252971	-0.794960
O	-2.591461	-0.613162	-1.060197
N	-2.000399	-0.075521	1.117945
O	-0.588932	-2.241490	-0.439320
H	0.273436	2.709985	-1.064447
H	-2.020476	1.869390	-1.150877
H	-1.213385	0.106366	1.722412
C	-3.089046	0.836065	1.398846
H	-3.446186	0.653574	2.408054
H	-3.902455	0.623132	0.712093
H	-2.824366	1.893026	1.310442
H	-2.603574	-1.561728	-0.899800
C	2.001745	-1.309674	0.327094
C	3.261279	-0.772877	0.513534
C	3.467718	0.580129	0.287396
C	2.425370	1.393790	-0.119389
H	1.807235	-2.360710	0.476287
H	4.079472	-1.401813	0.827017
H	4.451536	1.002832	0.422758
H	2.600425	2.442202	-0.309969

P-O3-7

C	-1.589495	0.151281	-0.452445
C	-0.508614	-0.895611	-0.118530
C	0.893633	-0.464750	-0.033756
C	1.190757	0.898113	0.054328
C	0.116991	1.882273	0.038844
C	-1.155551	1.552144	-0.149584
O	-1.759532	-0.005742	-1.839686
N	-2.839930	-0.148379	0.178157
O	-0.849703	-2.040270	0.054571
H	0.395304	2.917248	0.177440
H	-1.933385	2.302876	-0.175720
H	-3.047428	-1.110424	-0.053998
C	-2.854921	0.009697	1.617624
H	-3.839527	-0.256960	1.988617
H	-2.671857	1.048789	1.878058
H	-2.114778	-0.609054	2.132585
H	-2.589122	0.422714	-2.058218
C	1.903376	-1.413311	0.000509
C	3.222856	-1.016644	0.104163
C	3.526610	0.333818	0.191814
C	2.519966	1.282605	0.173110
H	1.629809	-2.455357	-0.059146
H	4.011836	-1.751981	0.119711
H	4.555141	0.649350	0.278060
H	2.763754	2.331869	0.249970

P-O3-8

C	1.512024	0.052613	0.125070
C	0.383078	-0.951753	-0.143675
C	-1.004823	-0.465006	-0.062503
C	-1.259310	0.907513	-0.126051
C	-0.151597	1.846396	-0.248699
C	1.119670	1.466698	-0.169361
O	1.768676	-0.063585	1.530650
N	2.634968	-0.359533	-0.624009
O	0.648786	-2.111502	-0.341260
H	-0.400047	2.884372	-0.417704
H	1.918446	2.185908	-0.265000
H	2.667299	-1.367532	-0.619032
C	3.904608	0.230136	-0.271286
H	4.677186	-0.234437	-0.875864
H	4.159433	0.112428	0.782151
H	3.912608	1.291441	-0.509669
H	1.210996	0.548336	2.010100
C	-2.046562	-1.374191	0.025574
C	-3.353563	-0.927356	0.070169
C	-3.614842	0.433218	0.007443
C	-2.577707	1.343053	-0.095898
H	-1.806972	-2.425817	0.057246
H	-4.166062	-1.632492	0.148079
H	-4.634151	0.786901	0.034486
H	-2.789057	2.400397	-0.156539

P-O3-9

C	-1.584968	0.453574	-0.227403
C	-0.572157	-0.666148	-0.494876
C	0.849736	-0.406258	-0.188420
C	1.297490	0.899717	0.026125
C	0.351094	2.004684	-0.027811
C	-0.955680	1.811924	-0.160544
O	-2.529353	0.383528	-1.247916
N	-2.244780	0.229062	1.041842
O	-0.954876	-1.751498	-0.854163
H	0.750423	3.006487	0.040033
H	-1.644694	2.643370	-0.198591
H	-1.687872	0.571311	1.806916
C	-2.788926	-1.091063	1.287381
H	-3.498256	-1.024595	2.107600
H	-2.039358	-1.847267	1.526052
H	-3.313654	-1.423856	0.397837
H	-3.312566	0.831143	-0.925026
C	1.741580	-1.466840	-0.170209
C	3.082183	-1.243526	0.080573
C	3.532779	0.050122	0.296734
C	2.649018	1.113798	0.264257
H	1.358653	-2.458039	-0.358076
H	3.775111	-2.069913	0.103870
H	4.579688	0.231251	0.486541
H	3.006936	2.120529	0.421728

P-O3-10

C	-1.565040	0.423905	-0.213305
C	-0.547084	-0.697987	-0.442909
C	0.874224	-0.419593	-0.154923
C	1.317601	0.891963	0.025815
C	0.365984	1.989238	-0.042423
C	-0.938979	1.784652	-0.162295
O	-2.469873	0.340804	-1.284269
N	-2.135595	0.159479	1.076653
O	-0.923309	-1.789601	-0.787594
H	0.757736	2.994940	0.007273
H	-1.625428	2.621041	-0.211364
H	-2.512168	0.995483	1.490052
C	-3.030667	-0.971710	1.197784
H	-3.416979	-0.988848	2.212282
H	-2.489591	-1.895812	1.024997
H	-3.864919	-0.942056	0.496164
H	-3.122459	1.033821	-1.192015
C	1.771522	-1.474556	-0.120286
C	3.112775	-1.238739	0.114730
C	3.559316	0.061389	0.297611
C	2.669768	1.119131	0.247335
H	1.392726	-2.472049	-0.280404
H	3.809529	-2.061395	0.152682
H	4.606641	0.251668	0.475691
H	3.023010	2.131071	0.380161

P-O4-1

C	-1.107394	-0.795926	0.373110
C	0.384748	-0.763708	0.177526
C	1.083549	0.431780	0.035332
C	0.367310	1.706439	-0.013600
C	-1.099911	1.675542	0.071109
C	-1.768859	0.536213	0.236124
O	0.914068	2.788151	-0.139318
H	-2.846075	0.569784	0.304908
O	-1.682906	2.873383	-0.032709
N	-1.686811	-1.838632	-0.454219
H	-1.603409	-1.583748	-1.426151
H	-0.965065	3.511854	-0.132274
H	-1.271809	-1.124531	1.406684
C	-3.046432	-2.191021	-0.127840
H	-3.364086	-3.010099	-0.766592
H	-3.085818	-2.543521	0.901219
H	-3.774845	-1.381138	-0.233782
C	2.469351	0.436237	-0.096695
C	3.164829	-0.751550	-0.092219
C	2.471954	-1.949452	0.037308
C	1.097357	-1.955551	0.169281
H	2.968366	1.386505	-0.205992
H	4.238712	-0.753649	-0.194813
H	3.010913	-2.884713	0.032724
H	0.552491	-2.882605	0.253196

P-O4-2

C	-0.295453	1.391891	-0.748025
C	0.756537	0.358657	-0.408840
C	0.423540	-0.937080	-0.025771
C	-0.981553	-1.337504	0.077336
C	-2.010291	-0.332834	-0.223080
C	-1.694151	0.911019	-0.576435
O	-1.342245	-2.454382	0.404514
H	-2.472766	1.634700	-0.765154
O	-3.265772	-0.772668	-0.093715
N	-0.145380	2.661933	-0.061668
H	-3.199418	-1.697241	0.176171
H	-0.172634	1.618050	-1.812038
H	0.664923	3.153066	-0.398916
C	-0.133293	2.574359	1.379953
H	0.674323	1.955560	1.783502
H	-1.077930	2.157648	1.721170
H	-0.044590	3.573657	1.795465
C	1.410023	-1.873675	0.268925
C	2.738972	-1.523928	0.187403
C	3.082634	-0.232371	-0.192178
C	2.101818	0.693924	-0.487171
H	1.100780	-2.865875	0.558863
H	3.507567	-2.245359	0.416058
H	4.122143	0.050410	-0.259101
H	2.386703	1.693500	-0.783423

P-O4-3

C	0.138244	-1.437035	0.506319
C	0.753700	-0.068778	0.338166
C	-0.007119	1.023058	-0.076821
C	-1.463619	0.902100	-0.182278
C	-2.082274	-0.367039	0.231696
C	-1.350100	-1.422295	0.580715
O	-2.191792	1.804821	-0.553799
H	-1.831758	-2.354852	0.830787
O	-3.418459	-0.362809	0.206207
N	0.476715	-2.389341	-0.541756
H	-3.678862	0.513698	-0.103289
H	0.529978	-1.860234	1.435469
H	0.081285	-2.085200	-1.417021
C	1.860378	-2.759576	-0.688097
H	2.236030	-3.124565	0.266843
H	2.519995	-1.956407	-1.028566
H	1.929495	-3.578819	-1.398637
C	0.578509	2.263078	-0.300588
C	1.932140	2.432242	-0.101042
C	2.693020	1.363561	0.350315
C	2.108182	0.129646	0.572193
H	-0.055362	3.079444	-0.610453
H	2.391986	3.392910	-0.271861
H	3.747436	1.495479	0.539671
H	2.708421	-0.685935	0.946626

P-O4-4

C	-0.962477	-0.980678	0.416865
C	0.503845	-0.702885	0.240904
C	0.987600	0.570735	-0.036200
C	0.068442	1.708717	-0.098771
C	-1.353774	1.460259	0.173285
C	-1.820175	0.238461	0.414785
O	0.421461	2.848533	-0.342407
H	-2.875584	0.111625	0.601596
O	-2.118600	2.556027	0.151601
N	-1.402604	-1.897724	-0.626245
H	-0.691109	-2.591025	-0.785317
H	-1.529470	3.291040	-0.059592
H	-1.078512	-1.451982	1.407984
C	-2.668986	-2.533045	-0.359498
H	-2.846077	-3.300511	-1.106783
H	-2.728282	-2.995212	0.634052
H	-3.479363	-1.813486	-0.443680
C	2.348176	0.793236	-0.219985
C	3.237971	-0.253933	-0.127040
C	2.766490	-1.526909	0.164849
C	1.414757	-1.745338	0.349124
H	2.676073	1.799353	-0.430383
H	4.293731	-0.085675	-0.270180
H	3.458276	-2.350278	0.255897
H	1.064440	-2.737980	0.596670

P-O4-5

C	-0.365728	1.342946	-0.751363
C	0.742272	0.389967	-0.395381
C	0.488338	-0.929267	-0.040038
C	-0.887798	-1.449855	0.072457
C	-1.982660	-0.486781	-0.178803
C	-1.730929	0.771827	-0.536202
O	-1.125335	-2.597596	0.366047
H	-2.558023	1.449842	-0.716905
O	-3.200013	-1.023509	-0.009901
N	-0.150422	2.624974	-0.104196
H	-3.873893	-0.369150	-0.184821
H	-0.269599	1.539184	-1.823975
H	-0.732941	3.326034	-0.531352
C	-0.327078	2.612897	1.329761
H	0.412483	1.951837	1.775813
H	-1.315891	2.277777	1.657120
H	-0.152757	3.612121	1.717509
C	1.539420	-1.796533	0.244860
C	2.840746	-1.351111	0.184029
C	3.097606	-0.029014	-0.158457
C	2.057816	0.832785	-0.444301
H	1.298833	-2.812672	0.515724
H	3.655484	-2.022524	0.406367
H	4.115224	0.328785	-0.199809
H	2.244788	1.865635	-0.694839

P-O4-6

C	-0.351442	1.371902	-0.747098
C	0.744138	0.386339	-0.416939
C	0.465475	-0.916820	-0.023066
C	-0.922890	-1.407174	0.094162
C	-1.995235	-0.439012	-0.217049
C	-1.721425	0.812702	-0.581559
O	-1.180909	-2.538507	0.430950
H	-2.523788	1.512361	-0.778400
O	-3.224856	-0.957108	-0.078403
N	-0.272684	2.636288	-0.035432
H	-3.882554	-0.295185	-0.284262
H	-0.239666	1.625510	-1.805504
H	0.507039	3.177172	-0.369443
C	-0.234165	2.519697	1.404243
H	0.618660	1.948753	1.783346
H	-1.142599	2.031521	1.749144
H	-0.207981	3.513962	1.840130
C	1.496730	-1.803865	0.271138
C	2.809146	-1.397741	0.177904
C	3.096117	-0.096753	-0.215041
C	2.072549	0.781785	-0.509226
H	1.232336	-2.806181	0.570213
H	3.608882	-2.084495	0.407132
H	4.121844	0.230103	-0.293097
H	2.308739	1.791019	-0.816433

P-O4-7

C	-1.041450	-0.862380	0.383979
C	0.443252	-0.735506	0.184721
C	1.058718	0.501589	0.031218
C	0.279332	1.753376	-0.016497
C	-1.191214	1.618021	0.066019
C	-1.773692	0.432385	0.242358
O	0.799290	2.837919	-0.132002
H	-2.853091	0.380993	0.314090
O	-1.830462	2.791293	-0.051598
N	-1.558482	-1.932248	-0.449195
H	-1.467303	-1.681179	-1.421252
H	-2.774176	2.658503	0.016675
H	-1.191179	-1.202458	1.415586
C	-2.900388	-2.357466	-0.142698
H	-3.162668	-3.196784	-0.780375
H	-2.937576	-2.705197	0.888147
H	-3.672914	-1.590908	-0.265991
C	2.440676	0.588549	-0.109564
C	3.210984	-0.552553	-0.101669
C	2.598754	-1.791633	0.041504
C	1.228384	-1.881511	0.181897
H	2.877031	1.568099	-0.227370
H	4.282162	-0.485459	-0.211727
H	3.195904	-2.690875	0.041056
H	0.742434	-2.839927	0.276721

P-O4-8

C	0.028848	1.432681	-0.499018
C	0.749428	0.118486	-0.343885
C	0.075024	-1.025871	0.073333
C	-1.395766	-1.037798	0.212946
C	-2.109697	0.180832	-0.230136
C	-1.451274	1.283396	-0.584131
O	-1.998661	-1.995921	0.634159
H	-1.994028	2.180419	-0.851145
O	-3.443455	0.041246	-0.211292
N	0.275907	2.398875	0.562848
H	-3.860834	0.859286	-0.475372
H	0.385761	1.901167	-1.420073
H	-0.078123	2.036731	1.434199
C	1.623113	2.887738	0.710795
H	1.960749	3.298544	-0.239651
H	2.351406	2.139772	1.035723
H	1.623922	3.698611	1.434193
C	0.760454	-2.214893	0.289170
C	2.121548	-2.279008	0.077116
C	2.795741	-1.154865	-0.376498
C	2.113876	0.029598	-0.588369
H	0.194141	-3.077179	0.605327
H	2.654438	-3.202429	0.241780
H	3.855745	-1.204170	-0.574029
H	2.644633	0.892751	-0.961765

P-O4-9

C	-0.941725	-0.986437	0.404026
C	0.519321	-0.687524	0.236138
C	0.981328	0.594369	-0.030759
C	0.058199	1.743890	-0.107788
C	-1.367622	1.463924	0.162378
C	-1.804912	0.229325	0.400359
O	0.439789	2.861220	-0.362428
H	-2.859716	0.069779	0.583479
O	-2.129078	2.567789	0.132534
N	-1.375396	-1.904521	-0.640315
H	-0.636437	-2.555561	-0.845234
H	-3.044962	2.337665	0.277351
H	-1.058564	-1.461502	1.392743
C	-2.597548	-2.606157	-0.341046
H	-2.774042	-3.358770	-1.103475
H	-2.593514	-3.098834	0.639660
H	-3.443993	-1.923636	-0.367756
C	2.340333	0.832939	-0.204151
C	3.245105	-0.201603	-0.110223
C	2.792232	-1.483328	0.171575
C	1.442557	-1.719876	0.344919
H	2.653718	1.844731	-0.409146
H	4.299092	-0.015973	-0.245708
H	3.495016	-2.297316	0.262863
H	1.101883	-2.718142	0.584018

Water Dimer

O	-1.504655	0.000000	-0.118662
O	1.369238	0.000000	0.099668
H	-1.901095	0.000002	0.747288
H	-0.553972	0.000000	0.019877
H	1.769198	-0.764627	-0.307607
H	1.769198	0.764626	-0.307610

Cartesian coordinates of transition states

TS-H1-1a

C	-0.516859	-0.307356	-0.316036
C	0.957143	-0.617210	-0.254347
C	1.908876	0.378974	-0.096969
C	1.513516	1.811151	-0.110829
C	0.129263	2.112048	-0.397668
C	-0.816334	1.167170	-0.535630
O	-1.161602	-1.166681	-1.097029
O	2.340018	2.681033	0.089174
N	-1.054619	-0.590364	1.147112
H	-0.136687	3.150687	-0.512148
O	-2.070359	1.502425	-0.743608
H	-0.886468	-1.585612	1.253465
C	-0.489426	0.155241	2.275396
H	-2.090047	-0.486513	1.146576
H	-2.295082	-0.950861	-1.277588
O	-3.441312	-0.550049	-1.313571
O	-3.817729	-0.622082	1.243868
H	-3.953890	-0.676578	0.270453
H	-4.382019	0.075872	1.565374
H	-3.886217	-0.708952	-2.140832
C	1.350931	-1.944556	-0.315502
C	2.689542	-2.273971	-0.199782
C	3.641026	-1.278863	-0.028076
C	3.251266	0.045024	0.013740
H	0.602959	-2.702582	-0.493197
H	2.993623	-3.307904	-0.256615
H	4.685012	-1.538010	0.056816
H	3.964310	0.847227	0.124056
H	-2.673220	0.757348	-1.050077
H	-0.931268	-0.211288	3.195398
H	0.585699	0.020321	2.299597
H	-0.720161	1.206301	2.152478

TS-H1-1b

C	-0.521360	-0.283989	-0.294697
C	0.952257	-0.602943	-0.261406
C	1.908766	0.383388	-0.081215
C	1.521024	1.816709	-0.056285
C	0.137923	2.128547	-0.330764
C	-0.814485	1.194165	-0.487491
O	-1.104690	-1.107974	-1.216487
O	2.352623	2.677285	0.160108
N	-1.092795	-0.670313	1.062314
H	-0.125704	3.170058	-0.419942
O	-2.060164	1.550750	-0.700605
H	-0.845762	-1.649329	1.162680
C	-0.598822	0.078026	2.220533
H	-2.267960	-0.661247	1.106366
H	-2.074102	-0.940467	-1.322808
O	-3.592066	-0.397971	-1.162727
O	-3.583106	-0.786635	1.153702
H	-3.785671	-0.633412	0.017300
H	-4.055531	-0.141711	1.674289
H	-4.301933	-0.503469	-1.787917
C	1.342035	-1.930821	-0.352847
C	2.679412	-2.267873	-0.251085
C	3.635543	-1.281604	-0.057056
C	3.249890	0.041235	0.020075
H	0.596947	-2.689487	-0.539968
H	2.977870	-3.301598	-0.333817
H	4.678538	-1.546903	0.019514
H	3.964753	0.838506	0.151761
H	-2.704916	0.828111	-0.973603
H	-0.999162	-0.380338	3.118325
H	-0.947653	1.101995	2.155112
H	0.485980	0.068808	2.258004

TS-H1-2a

C	0.489996	-0.214651	0.324072
C	-0.990155	-0.501860	0.303804
C	-1.900183	0.483876	-0.053362
C	-1.457804	1.893170	-0.228743
C	-0.105926	2.208948	0.171618
C	0.792819	1.270092	0.525985
O	1.153402	-1.073279	1.081293
O	-2.230846	2.735683	-0.644996
N	0.971212	-0.419199	-1.179723
H	0.165597	3.251181	0.218025
O	1.994532	1.609430	0.919368
C	0.866501	-1.804569	-1.651851
H	0.447127	0.213763	-1.774079
H	1.974394	-0.147703	-1.238974
H	2.280664	-0.866234	1.209053
O	3.436904	-0.446186	1.216755
O	3.702599	-0.189739	-1.343895
H	3.870582	-0.346707	-0.385306
H	4.209727	0.578072	-1.593885
H	3.942601	-0.682632	1.988641
C	-1.435093	-1.779467	0.597671
C	-2.784265	-2.076119	0.508607
C	-3.691125	-1.100538	0.122329
C	-3.249922	0.180079	-0.149455
H	-0.715669	-2.518181	0.913822
H	-3.130291	-3.069954	0.748078
H	-4.741978	-1.335856	0.053957
H	-3.929741	0.973065	-0.419913
H	2.614238	0.850977	1.151192
H	1.461887	-1.913398	-2.550824
H	-0.169968	-2.050604	-1.844747
H	1.260561	-2.442434	-0.869216

TS-H1-2b

C	-0.501799	-0.222376	-0.294203
C	0.981202	-0.495661	-0.311703
C	1.877406	0.497409	0.059212
C	1.414775	1.897324	0.254781
C	0.067558	2.200617	-0.169869
C	-0.814332	1.252413	-0.537885
O	-1.119471	-1.096466	-1.133060
O	2.170059	2.742815	0.695256
N	-1.002453	-0.468150	1.127426
H	-0.212014	3.239783	-0.230701
O	-1.994412	1.584382	-0.997059
H	-0.526156	0.192482	1.731374
C	-0.799702	-1.835332	1.617660
H	-2.156699	-0.258325	1.232128
H	-2.097804	-0.951812	-1.188093
O	-3.591694	-0.379886	-1.021943
O	-3.472847	-0.235165	1.323302
H	-3.723172	-0.328849	0.185977
H	-3.851136	0.560175	1.690636
H	-4.346489	-0.587985	-1.563243
C	1.447000	-1.761495	-0.625464
C	2.801821	-2.035987	-0.547621
C	3.694161	-1.053351	-0.148055
C	3.231607	0.214359	0.147605
H	0.745591	-2.515325	-0.944995
H	3.161879	-3.020389	-0.804422
H	4.748865	-1.272476	-0.086809
H	3.898043	1.014213	0.430736
H	-2.653683	0.843532	-1.140760
H	0.247888	-2.029433	1.816916
H	-1.161845	-2.520753	0.860311
H	-1.387356	-1.960733	2.520243

TS-H1-3a

C	-0.517654	-0.275361	-0.316993
C	0.949052	-0.622721	-0.254205
C	1.926210	0.345793	-0.083417
C	1.569846	1.788384	-0.083208
C	0.193249	2.127905	-0.356116
C	-0.779723	1.211432	-0.499152
O	-1.176931	-1.101767	-1.120258
O	2.422016	2.632583	0.120253
N	-1.060991	-0.582619	1.144490
H	-0.048906	3.174729	-0.445773
O	-2.025364	1.586378	-0.677135
H	-0.784529	-1.548686	1.283495
C	-0.603051	0.250923	2.260404
H	-2.099143	-0.593967	1.118510
H	-2.297726	-0.840595	-1.318837
O	-3.432483	-0.405815	-1.347982
O	-3.842666	-0.695663	1.181883
H	-3.980294	-0.640396	0.209316
H	-4.387673	-1.402468	1.514861
H	-3.860749	-0.448444	-2.197900
C	1.309609	-1.959291	-0.334364
C	2.638846	-2.324646	-0.221861
C	3.615375	-1.356715	-0.035021
C	3.259434	-0.024228	0.023953
H	0.543060	-2.695323	-0.526103
H	2.916289	-3.365157	-0.293627
H	4.652177	-1.643951	0.047450
H	3.992250	0.758395	0.144820
H	-2.654158	0.866070	-0.994596
H	-0.962148	-0.175225	3.190573
H	0.480697	0.290491	2.263517
H	-1.005938	1.248286	2.138653

TS-H1-3b

C	-0.521074	-0.252150	-0.292513
C	0.945472	-0.605083	-0.262438
C	1.924753	0.355522	-0.069122
C	1.573373	1.798147	-0.031842
C	0.197217	2.145045	-0.290203
C	-0.780934	1.236825	-0.446500
O	-1.117431	-1.040307	-1.239211
O	2.429308	2.634604	0.185276
N	-1.097914	-0.664399	1.056971
H	-0.045341	3.193440	-0.353875
O	-2.019731	1.626230	-0.624223
H	-0.746110	-1.605990	1.193386
C	-0.719217	0.161601	2.207359
H	-2.264360	-0.782068	1.059522
H	-2.070685	-0.827477	-1.373022
O	-3.597372	-0.253332	-1.170956
O	-3.588473	-0.875401	1.092526
H	-3.791329	-0.613078	-0.027092
H	-3.957762	-1.720468	1.335134
H	-4.341116	-0.143059	-1.754967
C	1.305187	-1.940685	-0.375184
C	2.633792	-2.310600	-0.276716
C	3.612284	-1.349851	-0.066017
C	3.257247	-0.019834	0.028983
H	0.543524	-2.679097	-0.577293
H	2.908105	-3.349590	-0.375853
H	4.648570	-1.640772	0.008443
H	3.990008	0.759116	0.171463
H	-2.692643	0.919997	-0.888778
H	-1.071285	-0.327247	3.108861
H	-1.201133	1.127589	2.118246
H	0.357949	0.291512	2.254891

TS-H1-4a

C	-0.501149	-0.196231	-0.313475
C	0.976243	-0.499092	-0.315157
C	1.898581	0.469959	0.054593
C	1.470818	1.880145	0.260526
C	0.123272	2.216547	-0.133019
C	-0.787997	1.294429	-0.505067
O	-1.182342	-1.050898	-1.060516
O	2.255146	2.704592	0.692453
N	-0.963034	-0.404351	1.197966
H	-0.137568	3.261971	-0.164152
O	-1.976862	1.654912	-0.906485
C	-0.787123	-1.777013	1.682792
H	-0.471045	0.263235	1.782063
H	-1.976030	-0.189503	1.258558
H	-2.289881	-0.812638	-1.219816
O	-3.444894	-0.359795	-1.252337
O	-3.716875	-0.209225	1.304192
H	-3.904139	-0.316023	0.343180
H	-4.389603	-0.664346	1.800694
H	-3.929766	-0.518412	-2.056706
C	1.406283	-1.774341	-0.640047
C	2.753359	-2.085521	-0.569333
C	3.672603	-1.127302	-0.169362
C	3.245843	0.151409	0.133434
H	0.677278	-2.499770	-0.964801
H	3.087802	-3.077064	-0.833545
H	4.721681	-1.373976	-0.114865
H	3.935132	0.932252	0.415070
H	-2.619365	0.908583	-1.134541
H	-1.360630	-1.904758	2.593773
H	0.261805	-1.973344	1.863880
H	-1.162228	-2.440377	0.911673

TS-H1-4b

C	-0.515446	-0.199413	-0.282858
C	0.964439	-0.489754	-0.326627
C	1.876107	0.482318	0.060379
C	1.431762	1.882574	0.294594
C	0.088248	2.211645	-0.118829
C	-0.808960	1.283906	-0.506030
O	-1.152633	-1.064559	-1.118101
O	2.201091	2.705929	0.752799
N	-1.001711	-0.456791	1.143265
H	-0.179590	3.254849	-0.156910
O	-1.977201	1.640338	-0.967307
H	-0.595143	0.256374	1.738498
C	-0.689745	-1.791808	1.659725
H	-2.164790	-0.355229	1.229669
H	-2.118526	-0.882613	-1.213340
O	-3.615421	-0.277585	-1.058227
O	-3.489834	-0.292924	1.286907
H	-3.749755	-0.320515	0.144940
H	-3.957233	-0.952130	1.792187
H	-4.389831	-0.292884	-1.611576
C	1.412501	-1.751046	-0.682069
C	2.764916	-2.042819	-0.627430
C	3.672672	-1.082308	-0.209395
C	3.227669	0.181790	0.126342
H	0.699710	-2.487991	-1.015382
H	3.110822	-3.023196	-0.917036
H	4.725396	-1.314852	-0.165903
H	3.905903	0.966425	0.423746
H	-2.663335	0.915340	-1.096054
H	0.370330	-1.902330	1.854678
H	-1.002670	-2.519599	0.919209
H	-1.252285	-1.944213	2.575041

TS-H1-5

C	-0.587831	0.495589	-0.362564
C	-0.019133	1.877204	-0.641090
C	1.197532	2.246260	-0.224434
C	2.130223	1.255155	0.282973
C	1.772522	-0.178241	0.075265
C	0.498011	-0.550019	-0.343766
O	-1.623332	0.307655	-1.204422
O	3.195461	1.560981	0.780443
N	-1.108079	0.536377	1.075735
O	-0.878834	2.689685	-1.225246
H	1.546022	3.260481	-0.329270
C	-2.109715	1.572468	1.340837
H	-0.310381	0.663740	1.688268
H	-1.592316	-0.483923	1.337684
H	-2.263684	-0.582314	-1.036961
O	-2.971445	-1.624734	-0.723989
O	-2.360795	-1.564441	1.560335
H	-2.763922	-1.708363	0.476016
H	-1.920460	-2.349371	1.876320
H	-3.890573	-1.594855	-0.973488
C	0.224341	-1.871363	-0.648832
C	1.225345	-2.821403	-0.525253
C	2.488633	-2.460306	-0.084480
C	2.763051	-1.138572	0.211359
H	-0.760288	-2.154681	-0.988096
H	1.015628	-3.849525	-0.777676
H	3.261562	-3.206883	0.012541
H	3.741990	-0.817545	0.531760
H	-1.598286	2.114577	-1.539681
H	-2.512876	1.411867	2.334319
H	-1.675375	2.564033	1.266439
H	-2.906812	1.464323	0.614626

TS-H1-6

C	-0.534905	-0.696574	0.340332
C	0.326721	-1.918446	0.581657
C	1.637612	-1.961107	0.333818
C	2.356397	-0.756360	-0.041703
C	1.629523	0.537175	0.084937
C	0.262826	0.579097	0.344940
O	-1.572059	-0.782677	1.203826
O	3.520632	-0.782376	-0.386932
N	-1.120236	-0.875276	-1.065654
O	-0.381987	-2.972554	0.962743
H	2.201428	-2.872628	0.446710
H	-1.620035	-1.757900	-1.031627
C	-0.212219	-0.863768	-2.214427
H	-1.925575	-0.078511	-1.250991
H	-2.410318	-0.059489	1.109713
O	-3.379404	0.773695	0.888040
O	-2.988170	0.748742	-1.441674
H	-3.321862	0.841092	-0.330976
H	-2.836987	1.603815	-1.835908
H	-4.226181	0.511479	1.237821
C	-0.362487	1.797491	0.552870
C	0.374449	2.967917	0.485273
C	1.730914	2.930201	0.203283
C	2.357867	1.714919	0.009343
H	-1.414788	1.832605	0.789487
H	-0.114480	3.913721	0.661535
H	2.299135	3.845985	0.151284
H	3.415897	1.644676	-0.189548
H	-1.205371	-2.604377	1.326462
H	-0.800629	-1.030993	-3.110135
H	0.262050	0.108483	-2.279242
H	0.547081	-1.632938	-2.124978

TS-H1-7

C	-0.579160	-0.497301	0.351182
C	0.012684	-1.864886	0.652844
C	1.239715	-2.217514	0.255693
C	2.160341	-1.215995	-0.254744
C	1.773572	0.211813	-0.071790
C	0.486803	0.568677	0.325921
O	-1.628766	-0.326350	1.179369
O	3.236058	-1.512164	-0.735447
N	-1.090163	-0.569636	-1.093710
O	-0.838395	-2.687219	1.238414
H	1.605536	-3.223314	0.381058
C	-2.014932	-1.672324	-1.363812
H	-0.282263	-0.632702	-1.702979
H	-1.639372	0.404026	-1.346473
H	-2.263151	0.569074	1.047715
O	-2.989887	1.617888	0.778800
O	-2.361363	1.548449	-1.493348
H	-2.815451	1.684998	-0.416397
H	-2.969442	1.694659	-2.211336
H	-3.898938	1.569823	1.059481
C	0.185904	1.890692	0.596879
C	1.172121	2.855000	0.468209
C	2.447745	2.508238	0.054672
C	2.749054	1.186292	-0.212570
H	-0.808588	2.170329	0.906645
H	0.937158	3.884673	0.688986
H	3.208343	3.266662	-0.047888
H	3.737216	0.876521	-0.515073
H	-1.567984	-2.120889	1.544647
H	-2.418778	-1.548816	-2.362862
H	-1.514323	-2.631237	-1.283202
H	-2.823071	-1.617340	-0.643556

TS-H1-8

C	-0.544948	-0.218130	-0.259692
C	0.915876	-0.604219	-0.201239
C	1.935164	0.331879	-0.106304
C	1.642687	1.784224	-0.150893
C	0.256248	2.174895	-0.330102
C	-0.734450	1.279176	-0.364715
O	-1.169754	-0.906727	-1.217762
O	2.527885	2.609491	-0.049249
N	-1.175822	-0.611272	1.083324
H	0.063907	3.234694	-0.417298
O	-2.026453	1.580290	-0.464462
H	-1.055688	-1.617780	1.118418
C	-0.623609	-0.001273	2.291477
H	-2.316416	-0.462664	1.059083
H	-2.318138	-0.783447	-1.331093
O	-3.553548	-0.739568	-1.349426
O	-3.681984	-0.491606	1.007435
H	-3.763055	-0.621795	-0.142691
H	-4.123167	0.314467	1.262303
H	-3.929091	-1.532331	-1.722940
C	1.231241	-1.953970	-0.241090
C	2.547958	-2.364096	-0.152625
C	3.565647	-1.426844	-0.036866
C	3.258680	-0.082396	-0.024884
H	0.437440	-2.672515	-0.384510
H	2.784595	-3.416460	-0.189624
H	4.593374	-1.748939	0.026548
H	4.023411	0.676029	0.038140
H	-2.152026	2.513880	-0.632934
H	-1.126315	-0.421170	3.155993
H	-0.804808	1.067505	2.263888
H	0.444604	-0.181088	2.362745

TS-H1-9

C	-0.489321	-0.208641	-0.360643
C	0.982337	-0.530838	-0.288192
C	1.901885	0.446574	0.075144
C	1.493710	1.871348	0.186057
C	0.166548	2.211704	-0.297009
C	-0.717823	1.266552	-0.642226
O	-1.146314	-1.045543	-1.159392
O	2.262509	2.714680	0.601884
N	-1.040876	-0.344240	1.087386
H	-0.053918	3.263883	-0.401170
O	-1.919927	1.478258	-1.148576
C	-1.187356	-1.735628	1.528686
H	-0.419631	0.162427	1.707603
H	-2.049086	0.113747	1.168078
H	-2.236588	-1.008636	-1.028227
O	-3.512883	-1.035968	-0.674278
O	-3.439032	0.508236	1.133512
H	-3.624568	-0.196127	0.248813
H	-4.014075	0.286184	1.860740
H	-4.078980	-0.840047	-1.415640
C	1.409677	-1.824463	-0.530082
C	2.747832	-2.146887	-0.379070
C	3.661054	-1.181457	0.016770
C	3.239704	0.116120	0.234049
H	0.685257	-2.553785	-0.857074
H	3.080366	-3.154266	-0.577527
H	4.702501	-1.437825	0.134253
H	3.928466	0.900289	0.507562
H	-2.134561	2.411081	-1.157735
H	-1.565589	-1.730416	2.545326
H	-0.234068	-2.249976	1.490848
H	-1.903705	-2.220459	0.876346

TS-H1-10

C	-0.562382	-0.546144	0.380233
C	0.066728	-1.919035	0.528022
C	1.322169	-2.190043	0.152275
C	2.241880	-1.146480	-0.268504
C	1.794872	0.253865	-0.078214
C	0.493128	0.542781	0.318969
O	-1.522141	-0.387212	1.292982
O	3.343833	-1.408897	-0.706086
N	-1.188034	-0.543454	-1.031831
O	-0.796842	-2.825060	0.974121
H	1.717520	-3.195167	0.180522
C	-2.260311	-1.526593	-1.234528
H	-0.447695	-0.677953	-1.711045
H	-1.635289	0.450865	-1.242917
H	-2.170717	0.457421	1.143570
O	-2.976549	1.508386	0.833157
O	-2.499811	1.573859	-1.492616
H	-2.843034	1.651581	-0.424088
H	-2.122780	2.400975	-1.779820
H	-3.870049	1.455450	1.158888
C	0.139662	1.851535	0.605918
C	1.079137	2.860465	0.476797
C	2.369576	2.576729	0.056978
C	2.728278	1.271789	-0.213390
H	-0.861862	2.079333	0.939172
H	0.799872	3.875858	0.713167
H	3.094938	3.369422	-0.041220
H	3.729557	1.005717	-0.514374
H	-0.363587	-3.673811	1.068454
H	-2.835836	-1.224340	-2.101919
H	-1.851219	-2.520053	-1.373957
H	-2.887931	-1.512939	-0.351421

TS-H1-11

C	-0.499359	-0.143406	-0.357043
C	0.960513	-0.525637	-0.279475
C	1.929775	0.403036	0.081585
C	1.596171	1.844092	0.195658
C	0.275073	2.247460	-0.257303
C	-0.663370	1.350616	-0.582191
O	-1.158222	-0.910653	-1.224779
O	2.408519	2.653018	0.595407
N	-1.090314	-0.331689	1.058221
H	0.101096	3.310461	-0.343075
O	-1.873634	1.649128	-1.040441
C	-1.254541	-1.734762	1.461666
H	-0.492922	0.153025	1.718068
H	-2.116768	0.115689	1.134356
H	-2.245189	-0.914121	-1.088556
O	-3.511513	-1.025268	-0.719577
O	-3.517185	0.313946	1.238717
H	-3.680620	-0.283377	0.278549
H	-3.845617	1.202105	1.133460
H	-4.144431	-0.917378	-1.422686
C	1.326182	-1.838334	-0.525195
C	2.646431	-2.226628	-0.377212
C	3.607878	-1.308186	0.016950
C	3.250784	0.007772	0.235286
H	0.567693	-2.531279	-0.853765
H	2.927709	-3.249090	-0.577826
H	4.635689	-1.615753	0.131241
H	3.977558	0.757724	0.506255
H	-1.956417	2.593484	-1.174433
H	-1.755024	-1.745422	2.423355
H	-0.292719	-2.229574	1.529076
H	-1.884781	-2.222171	0.727456

TS-H1-12

C	-0.548971	-0.551918	0.375607
C	0.060611	-1.939519	0.446841
C	1.315442	-2.210382	0.071472
C	2.259727	-1.164941	-0.287484
C	1.824417	0.232336	-0.065423
C	0.520339	0.523382	0.320284
O	-1.459251	-0.415004	1.346991
O	3.368080	-1.430407	-0.706532
N	-1.240083	-0.474179	-1.000282
O	-0.817073	-2.857144	0.843117
H	1.694603	-3.222138	0.058578
C	-2.415552	-1.343034	-1.161057
H	-0.543717	-0.676955	-1.708811
H	-1.595964	0.555426	-1.202886
H	-2.181375	0.333278	1.166504
O	-3.164856	1.221291	0.729675
O	-2.261802	1.836679	-1.364620
H	-2.807061	1.693886	-0.379378
H	-2.871947	1.991701	-2.079931
H	-3.548890	1.818238	1.364031
C	0.169551	1.831017	0.608929
C	1.111809	2.837858	0.503632
C	2.408702	2.550207	0.107041
C	2.765141	1.246966	-0.172906
H	-0.840955	2.058334	0.909120
H	0.829274	3.854046	0.730894
H	3.138813	3.340517	0.026675
H	3.768707	0.979925	-0.465077
H	-0.391364	-3.712391	0.907830
H	-2.903252	-1.074748	-2.091920
H	-2.129056	-2.386523	-1.172159
H	-3.085328	-1.148496	-0.332172

TS-H1-13

C	-0.559708	-0.546037	0.367776
C	0.093104	-1.904963	0.548090
C	1.355544	-2.161338	0.188160
C	2.260600	-1.108319	-0.242268
C	1.788187	0.285548	-0.075434
C	0.476967	0.560881	0.305063
O	-1.542654	-0.402574	1.256825
O	3.369935	-1.361036	-0.667267
N	-1.163555	-0.579096	-1.059185
O	-0.755397	-2.818264	1.010947
H	1.769177	-3.158078	0.242161
C	-2.146135	-1.645447	-1.279887
H	-0.403854	-0.643427	-1.727353
H	-1.685417	0.374899	-1.261636
H	-2.179770	0.456697	1.140715
O	-2.989880	1.517653	0.885461
O	-2.474806	1.572175	-1.426086
H	-2.868606	1.643076	-0.367779
H	-3.150925	1.705965	-2.082817
H	-3.874197	1.446334	1.231431
C	0.100969	1.868451	0.562555
C	1.027077	2.888833	0.426948
C	2.326205	2.618491	0.028812
C	2.707512	1.314813	-0.216503
H	-0.907263	2.094661	0.872795
H	0.725670	3.903788	0.634933
H	3.040143	3.420665	-0.076054
H	3.715687	1.059100	-0.502953
H	-0.302695	-3.653171	1.132878
H	-2.725208	-1.403597	-2.164345
H	-1.655246	-2.602965	-1.406276
H	-2.792126	-1.679378	-0.410323

TS-H2-1b

C	-0.177469	1.189861	-0.516751
C	0.873098	0.410064	-0.805396
C	0.801286	-1.068060	-0.673913
C	-0.472624	-1.626028	-0.059922
C	-1.647403	-0.774016	-0.054583
C	-1.480102	0.607060	-0.229718
O	-0.110129	2.531845	-0.506267
O	-0.432507	-2.747037	0.406559
H	0.726281	2.778547	-0.050603
N	1.930797	-1.545490	0.157740
H	1.577174	-2.367339	0.644985
H	2.165427	-0.737114	0.915647
O	2.225070	2.469859	0.714053
H	2.867498	3.141281	0.922534
H	2.379321	1.392087	1.348734
O	2.470221	0.331123	1.772381
H	2.081893	0.308198	2.643078
C	3.146697	-1.900330	-0.582757
H	3.908693	-2.196754	0.129310
H	3.476682	-1.029608	-1.133159
H	2.938844	-2.721239	-1.262680
H	0.889654	-1.539415	-1.658407
O	2.090265	0.839466	-1.161558
H	2.318085	1.635197	-0.593558
C	-2.597390	1.426428	-0.105034
C	-3.836978	0.877954	0.159687
C	-3.996504	-0.492670	0.331612
C	-2.893790	-1.313685	0.241369
H	-2.468905	2.490096	-0.218516
H	-4.694916	1.528299	0.240901
H	-4.969773	-0.906225	0.542627
H	-2.967826	-2.379099	0.396005

TS-H2-1a

C	-0.147582	1.189982	-0.502619
C	0.881192	0.362827	-0.782057
C	0.781487	-1.103607	-0.662047
C	-0.487713	-1.640444	-0.022898
C	-1.653574	-0.781809	-0.041549
C	-1.464696	0.594382	-0.230440
O	-0.054666	2.491272	-0.469876
O	-0.441049	-2.746176	0.482265
H	1.009329	2.741877	0.062751
N	1.917875	-1.616680	0.163572
H	1.536133	-2.414985	0.674209
H	2.167971	-0.860182	0.846435
O	2.081752	2.694170	0.542944
H	2.481374	3.552052	0.646747
H	2.419151	1.335688	1.429509
O	2.553896	0.447656	1.850814
H	2.210987	0.520925	2.737382
C	3.113277	-2.020211	-0.591744
H	3.881367	-2.323832	0.110158
H	3.446988	-1.168739	-1.169431
H	2.858026	-2.848862	-1.242985
H	0.867314	-1.597813	-1.636627
O	2.130585	0.744165	-1.150502
H	2.328863	1.610096	-0.735902
C	-2.572659	1.427205	-0.132030
C	-3.823639	0.897660	0.118971
C	-4.002962	-0.468977	0.307665
C	-2.909715	-1.305004	0.246178
H	-2.416532	2.486456	-0.256170
H	-4.675790	1.558300	0.177044
H	-4.984673	-0.867642	0.508539
H	-3.000274	-2.367296	0.413600

TS-H2-2a

C	0.088314	-1.254897	-0.597807
C	-0.927087	-0.448400	-0.967355
C	-0.887631	1.024110	-0.836139
C	0.391790	1.632271	-0.285505
C	1.534895	0.748692	-0.109126
C	1.376192	-0.634891	-0.249568
O	0.002629	-2.552734	-0.509714
O	0.409897	2.820017	-0.037389
H	-1.064111	-2.774499	0.030297
N	-2.061275	1.344496	0.046497
H	-2.801770	0.791258	-0.392388
H	-1.934153	0.845078	0.951136
O	-2.126133	-2.678154	0.522681
H	-2.541197	-3.521767	0.674551
H	-2.158514	-1.376445	1.566191
O	-2.122138	-0.511902	2.048831
H	-1.570973	-0.656008	2.813155
C	-2.479199	2.742733	0.208779
H	-3.414200	2.752673	0.757684
H	-1.715912	3.292753	0.739273
H	-2.618654	3.185828	-0.770715
H	-1.095896	1.529001	-1.783979
O	-2.179702	-0.865252	-1.317059
H	-2.390335	-1.677051	-0.801434
C	2.475388	-1.453373	-0.023813
C	3.698112	-0.903322	0.310035
C	3.852051	0.471997	0.444263
C	2.764994	1.294590	0.242783
H	2.336133	-2.518187	-0.116493
H	4.545309	-1.552887	0.471993
H	4.810938	0.890161	0.706900
H	2.838918	2.365752	0.350273

TS-H2-2b

C	0.094827	-1.261900	-0.612987
C	-0.936037	-0.492208	-0.981541
C	-0.902662	0.991626	-0.860205
C	0.396448	1.608454	-0.366028
C	1.526972	0.720102	-0.124527
C	1.369932	-0.666800	-0.237555
O	0.025527	-2.601818	-0.554065
O	0.450026	2.811489	-0.225695
H	-0.815838	-2.829964	-0.097736
N	-2.049971	1.305027	0.037724
H	-2.837464	0.879764	-0.446138
H	-1.986674	0.643683	0.954016
O	-2.277483	-2.441854	0.684218
H	-2.923085	-3.078086	0.976492
H	-2.207146	-1.415417	1.399298
O	-2.107178	-0.382817	1.901900
H	-1.469468	-0.431897	2.609122
C	-2.349515	2.705901	0.343109
H	-3.304879	2.732992	0.855764
H	-1.579535	3.119990	0.978102
H	-2.397313	3.290263	-0.569659
H	-1.112343	1.464979	-1.822693
O	-2.161595	-0.937545	-1.315335
H	-2.400640	-1.675033	-0.677777
C	2.462231	-1.482940	0.036026
C	3.675073	-0.926778	0.393484
C	3.828616	0.450594	0.498233
C	2.749925	1.269417	0.243613
H	2.336517	-2.550423	-0.037201
H	4.514488	-1.574843	0.595791
H	4.780455	0.873352	0.778105
H	2.823483	2.343005	0.322530

TS-H3-1

C	0.662653	-0.459878	-0.312316
C	-0.817260	-0.754162	-0.269831
C	-1.756069	0.250208	-0.069618
C	-1.331647	1.652588	-0.042411
C	0.091930	1.951676	-0.295188
C	1.000236	0.990588	-0.445961
O	1.269887	-1.254075	-1.211491
O	-2.092805	2.583914	0.137153
N	1.222114	-0.899404	1.070690
O	0.370851	3.253055	-0.373771
H	2.033090	1.220621	-0.665205
H	1.180558	-1.912564	1.039238
C	0.575392	-0.387662	2.276774
H	2.288399	-0.642358	1.094570
H	2.302004	-0.948464	-1.375330
O	3.558549	-0.487088	-1.365617
O	3.733888	-0.414491	1.007417
H	3.811145	-0.446511	-0.109489
H	4.154278	0.371125	1.345322
H	4.180301	-0.971329	-1.900360
C	-1.243083	-2.066337	-0.386749
C	-2.588751	-2.370447	-0.283071
C	-3.523611	-1.367234	-0.064600
C	-3.108440	-0.055867	0.031347
H	-0.513829	-2.833987	-0.596957
H	-2.914165	-3.394375	-0.385311
H	-4.571640	-1.610752	0.011888
H	-3.808958	0.752241	0.173861
H	-0.461464	3.721982	-0.235550
H	1.146602	-0.704845	3.142601
H	-0.442927	-0.752594	2.350824
H	0.570750	0.696274	2.235275

TS-H3-2

C	-0.633073	-0.327920	0.308100
C	0.833061	-0.686821	0.266298
C	1.794863	0.263405	-0.063200
C	1.422005	1.677231	-0.171488
C	0.038709	2.054476	0.179829
C	-0.892313	1.142386	0.450536
O	-1.285319	-1.096129	1.191184
O	2.201090	2.559827	-0.476370
N	-1.200444	-0.647867	-1.114555
O	-0.177392	3.369665	0.216693
H	-1.897687	1.423522	0.729240
C	-1.249479	-2.069477	-1.461184
H	-0.666067	-0.128539	-1.800559
H	-2.231151	-0.266477	-1.145961
H	-2.295466	-0.741125	1.343155
O	-3.533424	-0.200075	1.318964
O	-3.662311	0.018149	-1.046809
H	-3.757053	-0.072712	0.071605
H	-4.024634	0.848131	-1.343755
H	-4.205472	-0.653731	1.818331
C	1.230104	-1.986623	0.529427
C	2.564488	-2.338971	0.423979
C	3.516559	-1.398193	0.057762
C	3.133432	-0.093111	-0.172082
H	0.485570	-2.700923	0.843217
H	2.866483	-3.352544	0.639196
H	4.554710	-1.680159	-0.021546
H	3.851582	0.674567	-0.414895
H	0.657372	3.792550	-0.019906
H	-1.900749	-2.192757	-2.319304
H	-1.667689	-2.597081	-0.611965
H	-0.257915	-2.447442	-1.682112

TS-H3-3

C	0.661553	-0.462314	-0.294034
C	-0.819508	-0.754997	-0.257027
C	-1.760260	0.249761	-0.071757
C	-1.334797	1.652016	-0.041443
C	0.092966	1.948876	-0.266358
C	1.005012	0.988631	-0.400243
O	1.261668	-1.247276	-1.207831
O	-2.099589	2.582870	0.124821
N	1.219166	-0.932962	1.079878
O	0.375867	3.250082	-0.329784
H	2.044132	1.223995	-0.581590
H	1.103312	-1.940121	1.056081
C	0.632765	-0.366454	2.292761
H	2.297731	-0.741722	1.078258
H	2.277158	-0.921912	-1.402321
O	3.524782	-0.422402	-1.417531
O	3.706857	-0.342217	0.949878
H	3.797559	-0.393508	-0.168933
H	4.432520	-0.784421	1.379537
H	4.156875	-0.818339	-2.008574
C	-1.245449	-2.067330	-0.375964
C	-2.592035	-2.371128	-0.286376
C	-3.528789	-1.366802	-0.081821
C	-3.113775	-0.055453	0.014503
H	-0.515524	-2.836404	-0.579504
H	-2.916609	-3.395208	-0.389824
H	-4.577782	-1.609490	-0.016566
H	-3.815070	0.753780	0.146418
H	-0.457487	3.720103	-0.203664
H	1.156709	-0.762470	3.155850
H	-0.422121	-0.610236	2.357895
H	0.761668	0.709394	2.267920

TS-H3-4

C	0.637915	-0.316311	-0.287784
C	-0.825308	-0.691761	-0.243523
C	-1.805379	0.249153	0.057179
C	-1.456026	1.669790	0.147483
C	-0.069866	2.060765	-0.172646
C	0.880540	1.158653	-0.405506
O	1.282473	-1.070865	-1.186602
O	-2.253379	2.545367	0.423929
N	1.225777	-0.645160	1.126376
O	0.133942	3.377473	-0.206096
H	1.896156	1.461900	-0.609690
C	1.303956	-2.069990	1.449542
H	0.690133	-0.142875	1.824072
H	2.245550	-0.236717	1.147835
H	2.317079	-0.763426	-1.331182
O	3.600962	-0.412856	-1.294697
O	3.597900	0.299915	0.968341
H	3.749259	0.011121	-0.118629
H	4.342316	0.033222	1.499469
H	3.932610	0.135816	-1.998776
C	-1.202698	-2.000608	-0.494271
C	-2.532607	-2.370877	-0.398390
C	-3.502399	-1.438392	-0.058100
C	-3.140201	-0.124697	0.154604
H	-0.445719	-2.708018	-0.793545
H	-2.817287	-3.391763	-0.602403
H	-4.537403	-1.733816	0.013061
H	-3.871805	0.636938	0.375183
H	-0.709814	3.792175	0.012424
H	1.946225	-2.196785	2.314556
H	1.739687	-2.574827	0.594971
H	0.319835	-2.473462	1.657493

TS-H3-5

C	-0.400833	-0.769033	-0.445739
C	0.712346	-1.760779	-0.560402
C	1.969246	-1.480256	-0.228078
C	2.379349	-0.122434	0.185479
C	1.386535	0.949082	0.093739
C	0.076580	0.664719	-0.286708
O	-1.268045	-0.972621	-1.456507
O	3.533981	0.044437	0.528137
N	-1.116573	-1.076211	0.892026
H	0.437499	-2.742477	-0.912711
O	2.962029	-2.367225	-0.262534
C	-1.774165	-2.388148	0.934712
H	-0.428776	-1.008808	1.632967
H	-1.901659	-0.345649	1.123796
H	-2.195583	-0.513192	-1.316441
O	-3.444522	0.076535	-0.943573
O	-3.197771	0.295501	1.404680
H	-3.477337	0.242004	0.313496
H	-3.256326	1.190889	1.725078
H	-4.235632	-0.262509	-1.350880
C	-0.808906	1.710897	-0.488529
C	-0.391066	3.015857	-0.289956
C	0.906120	3.295364	0.114522
C	1.798510	2.260762	0.297820
H	-1.817794	1.505783	-0.816669
H	-1.085893	3.823801	-0.461300
H	1.220170	4.316100	0.266428
H	2.824364	2.438471	0.580622
H	3.757993	-1.898108	0.019083
H	-2.361269	-2.441179	1.844077
H	-2.431057	-2.455248	0.076578
H	-1.040367	-3.185593	0.908895

TS-H3-6

C	0.376880	-0.902487	0.466024
C	-0.852162	-1.737967	0.612307
C	-2.077770	-1.288146	0.363089
C	-2.321075	0.116355	-0.020849
C	-1.186236	1.040835	0.003954
C	0.095297	0.579925	0.300689
O	1.229043	-1.224771	1.457408
O	-3.460106	0.443306	-0.294287
N	1.049462	-1.362242	-0.852598
H	-0.685863	-2.758110	0.925309
O	-3.177213	-2.035926	0.444309
H	1.294921	-2.331893	-0.681009
C	0.287597	-1.240428	-2.096026
H	2.008090	-0.862890	-1.006411
H	2.218994	-0.836744	1.372288
O	3.504027	-0.374939	1.140652
O	3.415292	-0.452096	-1.234754
H	3.627680	-0.401999	-0.144390
H	3.659383	0.366620	-1.656759
H	4.184425	-0.817331	1.639354
C	1.126476	1.496763	0.425315
C	0.879229	2.845579	0.230754
C	-0.391617	3.298597	-0.089966
C	-1.427884	2.395036	-0.193105
H	2.114965	1.163220	0.705899
H	1.688747	3.550597	0.342532
H	-0.572763	4.351638	-0.238102
H	-2.436644	2.709709	-0.410661
H	-3.917473	-1.458824	0.216617
H	0.913211	-1.575224	-2.916094
H	-0.617610	-1.834463	-2.051497
H	0.032956	-0.197591	-2.248628

TS-H3-7

C	0.639316	-0.334342	-0.287120
C	-0.830421	-0.682063	-0.261470
C	-1.789114	0.273870	0.058735
C	-1.406757	1.684737	0.175167
C	-0.017058	2.051772	-0.157951
C	0.913082	1.134619	-0.415849
O	1.290704	-1.109255	-1.166074
O	-2.184091	2.570776	0.474606
N	1.196106	-0.669532	1.138054
O	0.209543	3.365039	-0.187039
H	1.926483	1.415162	-0.664396
C	1.176519	-2.088222	1.493021
H	0.695435	-0.115401	1.822242
H	2.242509	-0.337444	1.154804
H	2.290145	-0.743989	-1.349805
O	3.516524	-0.178677	-1.361413
O	3.627385	0.100116	0.992252
H	3.751445	-0.037556	-0.122901
H	4.372689	-0.234235	1.481080
H	4.193242	-0.566495	-1.906518
C	-1.235512	-1.976728	-0.538703
C	-2.573812	-2.319076	-0.452695
C	-3.522845	-1.372748	-0.093106
C	-3.131786	-0.072123	0.148255
H	-0.493573	-2.695306	-0.848750
H	-2.881126	-3.328740	-0.678577
H	-4.564282	-1.646430	-0.028983
H	-3.846404	0.700819	0.384730
H	-0.623252	3.794001	0.044392
H	1.814356	-2.241378	2.357140
H	1.570973	-2.639535	0.647001
H	0.168433	-2.418917	1.713806

TS-H3-8

C	0.634191	-0.505164	-0.308598
C	-0.853024	-0.738089	-0.288346
C	-1.738291	0.308377	-0.067474
C	-1.266560	1.707719	0.003394
C	0.161548	1.938333	-0.324763
C	1.018850	0.929589	-0.468858
O	1.238258	-1.330726	-1.185162
O	-2.001220	2.624325	0.279303
N	1.157036	-0.944093	1.089096
O	0.461210	3.234967	-0.457161
H	2.058335	1.094012	-0.724725
H	1.087901	-1.956064	1.067385
C	0.500683	-0.401443	2.277167
H	2.218966	-0.717374	1.128583
H	2.252170	-1.027732	-1.348706
O	3.531392	-0.517046	-1.332713
O	3.696869	-0.522530	1.048275
H	3.781130	-0.520075	-0.057778
H	4.174110	0.211122	1.423981
H	4.163915	-0.975230	-1.877988
C	-1.337632	-2.027639	-0.431692
C	-2.696339	-2.270011	-0.338388
C	-3.580148	-1.226787	-0.099004
C	-3.102103	0.061071	0.028679
H	-0.643505	-2.824645	-0.651422
H	-3.070196	-3.274685	-0.463399
H	-4.639180	-1.420127	-0.029316
H	-3.762749	0.898143	0.192450
H	1.378367	3.334133	-0.709626
H	1.057998	-0.707298	3.155945
H	-0.521798	-0.754748	2.343662
H	0.506173	0.681550	2.214250

TS-H3-9

C	0.625782	-0.530679	-0.297076
C	-0.865337	-0.737399	-0.275685
C	-1.733466	0.327261	-0.076778
C	-1.238110	1.719453	-0.018798
C	0.198921	1.920637	-0.321067
C	1.038233	0.895644	-0.456415
O	1.211645	-1.375184	-1.169453
O	-1.963044	2.651060	0.231752
N	1.142714	-0.975896	1.102695
O	0.530254	3.210584	-0.437989
H	2.085538	1.046595	-0.685078
H	1.027292	-1.983454	1.091963
C	0.519340	-0.388024	2.287296
H	2.210946	-0.780178	1.126384
H	2.221281	-1.086404	-1.352888
O	3.506738	-0.575480	-1.357209
O	3.641095	-0.351572	1.009102
H	3.753687	-0.475983	-0.094349
H	4.367990	-0.750218	1.477638
H	4.156606	-0.999900	-1.908123
C	-1.372134	-2.020322	-0.403847
C	-2.735261	-2.237977	-0.315544
C	-3.602014	-1.175890	-0.098091
C	-3.101925	0.105102	0.013233
H	-0.691427	-2.832576	-0.609762
H	-3.125772	-3.237769	-0.428318
H	-4.664731	-1.349552	-0.032616
H	-3.748332	0.956315	0.160053
H	1.462326	3.290711	-0.637866
H	1.055887	-0.720338	3.169245
H	-0.522620	-0.679431	2.354137
H	0.594646	0.691367	2.217737

TS-H3-10

C	0.625628	-0.523727	-0.311274
C	-0.864282	-0.736694	-0.267045
C	-1.738596	0.325397	-0.082344
C	-1.254371	1.721575	-0.051610
C	0.185201	1.928640	-0.339742
C	1.028357	0.906098	-0.468219
O	1.191882	-1.365258	-1.196826
O	-1.986713	2.653744	0.173639
N	1.176366	-0.956218	1.079558
O	0.512955	3.220564	-0.444860
H	2.081710	1.062805	-0.657512
H	1.126817	-1.969168	1.055694
C	0.521936	-0.420779	2.272734
H	2.227769	-0.684074	1.107108
H	2.232060	-1.153783	-1.337548
O	3.565619	-0.873193	-1.268608
O	3.631236	-0.147872	0.990381
H	3.765141	-0.447515	-0.081512
H	4.350416	-0.484451	1.517098
H	4.013218	-0.462811	-2.001123
C	-1.363488	-2.025111	-0.369135
C	-2.723999	-2.250590	-0.265196
C	-3.596852	-1.190565	-0.061413
C	-3.105104	0.095532	0.021073
H	-0.678791	-2.836050	-0.566309
H	-3.108013	-3.255160	-0.355452
H	-4.657747	-1.370382	0.015825
H	-3.756473	0.944937	0.155742
H	1.451224	3.308235	-0.607890
H	1.088617	-0.717303	3.148557
H	-0.495808	-0.786151	2.345660
H	0.518887	0.661843	2.207978

TS-H4-1

C	0.212924	1.247281	-0.612839
C	-0.884462	0.501302	-0.860078
C	-0.951484	-0.927648	-0.526688
C	0.237563	-1.440963	0.294581
C	1.509179	-0.735342	0.150630
C	1.491705	0.596437	-0.267108
O	0.208657	2.547313	-0.633339
O	0.078372	-2.412342	0.997873
H	-1.802703	1.001297	-1.129445
H	-0.790423	2.841008	-0.235988
N	-2.151987	-1.173841	0.318551
H	-1.952222	-2.012615	0.860328
H	-2.271388	-0.278706	0.994323
O	-1.955937	2.898000	0.339881
H	-2.205493	3.749011	0.686401
H	-2.283976	1.913921	1.050614
O	-2.562427	0.952648	1.614774
H	-2.329501	1.047475	2.534301
C	-3.410495	-1.317712	-0.417924
H	-4.211147	-1.423304	0.304814
H	-3.585369	-0.417877	-0.996419
H	-3.367177	-2.175725	-1.075443
O	-1.039662	-1.784249	-1.636265
H	-0.864900	-1.252445	-2.412317
C	2.696258	-1.348773	0.521663
C	3.881533	-0.644008	0.444279
C	3.867317	0.682146	0.034552
C	2.679227	1.307201	-0.303313
H	2.667824	-2.370660	0.866835
H	4.812334	-1.117805	0.713768
H	4.792041	1.237097	-0.010460
H	2.648413	2.345732	-0.591093

TS-H4-2

C	0.217375	1.244088	-0.613013
C	-0.890312	0.505360	-0.839896
C	-0.957215	-0.924524	-0.510484
C	0.226051	-1.438701	0.317974
C	1.501520	-0.742197	0.166489
C	1.492525	0.584257	-0.267369
O	0.225703	2.541648	-0.652892
O	0.061175	-2.406696	1.024216
H	-1.808961	1.006538	-1.107183
H	-0.771265	2.856921	-0.229118
N	-2.166714	-1.182727	0.319356
H	-1.953194	-2.003862	0.883080
H	-2.316673	-0.276897	0.966782
O	-1.896809	2.983425	0.370244
H	-1.921660	3.781631	0.890487
H	-2.238159	1.979599	1.019953
O	-2.531186	0.988591	1.548727
H	-3.206855	1.130832	2.204953
C	-3.405731	-1.373318	-0.437434
H	-4.217358	-1.498386	0.270498
H	-3.595341	-0.485353	-1.029868
H	-3.326115	-2.236989	-1.083810
O	-1.027031	-1.776760	-1.626042
H	-0.845314	-1.238374	-2.396033
C	2.685073	-1.360003	0.541153
C	3.875401	-0.665334	0.451041
C	3.869954	0.655293	0.023869
C	2.685359	1.284947	-0.317714
H	2.649951	-2.377266	0.899087
H	4.803429	-1.142720	0.723792
H	4.798722	1.202519	-0.031555
H	2.660970	2.320025	-0.618263

TS-H4-3

C	0.226182	1.239201	-0.636550
C	-0.880700	0.499917	-0.864855
C	-0.959012	-0.925301	-0.515525
C	0.217254	-1.431688	0.327627
C	1.497788	-0.746159	0.169379
C	1.497013	0.575636	-0.278970
O	0.240413	2.536711	-0.682898
O	0.042551	-2.383249	1.053953
H	-1.796628	1.001441	-1.138856
H	-0.724260	2.869385	-0.188208
N	-2.173739	-1.160803	0.309433
H	-1.971214	-1.974627	0.887303
H	-2.331449	-0.235970	0.949058
O	-1.766114	3.004319	0.523887
H	-2.404989	3.638822	0.214635
H	-2.250159	1.986145	1.032052
O	-2.661143	1.002445	1.492238
H	-2.690651	1.091320	2.440988
C	-3.409574	-1.359195	-0.451277
H	-4.229164	-1.433379	0.254119
H	-3.576512	-0.494867	-1.083876
H	-3.341814	-2.250378	-1.060852
O	-1.026777	-1.793731	-1.619003
H	-0.823228	-1.271583	-2.394583
C	2.676746	-1.365368	0.556434
C	3.870685	-0.677325	0.463600
C	3.873173	0.638988	0.023021
C	2.693071	1.270718	-0.330029
H	2.635389	-2.378239	0.926012
H	4.795301	-1.156019	0.745493
H	4.804614	1.181568	-0.033057
H	2.673722	2.303485	-0.638810

TS-H4-4

C	0.008899	1.051910	-0.976260
C	-1.029081	0.222479	-1.181348
C	-1.078089	-1.099081	-0.539015
C	0.275698	-1.668772	-0.099191
C	1.416305	-0.777108	-0.002558
C	1.280631	0.548835	-0.423904
O	-0.052039	2.341333	-1.195796
O	0.292154	-2.850480	0.179215
H	-1.940324	0.606237	-1.610077
H	-0.967044	2.658143	-0.667439
N	-1.836916	-0.932274	0.771290
H	-1.764043	-1.799318	1.294165
H	-1.425059	-0.072198	1.349039
O	-1.975991	2.722489	0.186801
H	-2.253574	3.605091	0.413449
H	-1.608101	1.996453	1.181617
O	-1.278379	1.227798	1.937110
H	-0.431396	1.482629	2.293352
C	-3.250921	-0.569769	0.574353
H	-3.754288	-0.640082	1.531381
H	-3.285795	0.460049	0.233267
H	-3.704856	-1.235599	-0.149357
O	-1.737783	-2.049318	-1.286809
H	-1.395669	-2.909633	-1.019761
C	2.624786	-1.250325	0.495358
C	3.706345	-0.399539	0.586658
C	3.573042	0.922281	0.179978
C	2.371984	1.396971	-0.316201
H	2.687929	-2.281369	0.807198
H	4.647425	-0.756295	0.974318
H	4.418465	1.589712	0.251815
H	2.253458	2.420234	-0.633389

TS-H4-5

C	0.132536	1.197832	-0.982132
C	-1.036485	0.579631	-1.240984
C	-1.330710	-0.751975	-0.679951
C	-0.090589	-1.605230	-0.408618
C	1.160799	-0.923952	-0.121391
C	1.266792	0.439374	-0.409869
O	0.329639	2.476701	-1.144943
O	-0.228737	-2.809240	-0.438450
H	-1.865713	1.138198	-1.647114
H	-0.519083	2.980847	-0.568510
N	-2.003507	-0.492193	0.662743
H	-2.895013	-0.092097	0.386446
H	-1.511580	0.364384	1.235010
O	-1.430462	3.254189	0.253273
H	-1.447241	4.164312	0.533508
H	-1.299136	2.413671	1.172762
O	-1.171903	1.527920	1.893835
H	-0.306583	1.571408	2.293024
C	-2.257947	-1.656645	1.513740
H	-2.900090	-1.350748	2.331984
H	-1.321594	-2.023537	1.917024
H	-2.737389	-2.445411	0.943599
O	-2.224208	-1.484296	-1.429229
H	-1.955840	-2.408275	-1.367652
C	2.240807	-1.637014	0.383527
C	3.432697	-0.987320	0.630918
C	3.540947	0.369820	0.356481
C	2.470655	1.079287	-0.160073
H	2.121682	-2.691963	0.576878
H	4.274242	-1.529488	1.032352
H	4.474345	0.878707	0.544183
H	2.541900	2.130305	-0.388484

TS-H4-6

C	0.151840	1.128084	-0.880555
C	-0.941519	0.370420	-1.096104
C	-1.062943	-0.994935	-0.568566
C	0.214423	-1.595225	0.035208
C	1.429288	-0.809362	0.073669
C	1.394746	0.517015	-0.363587
O	0.187868	2.414562	-1.073512
O	0.110657	-2.734783	0.448096
H	-1.820182	0.822503	-1.528014
H	-0.685811	2.850719	-0.448049
N	-2.038294	-0.970155	0.590699
H	-1.884422	-1.812106	1.138128
H	-1.868995	-0.027276	1.216975
O	-1.544220	3.111753	0.394844
H	-2.311386	3.570126	0.066459
H	-1.782140	2.144201	1.131607
O	-1.942529	1.212831	1.796441
H	-1.552791	1.363875	2.653091
C	-3.445912	-0.895195	0.183375
H	-4.055426	-0.878404	1.079342
H	-3.600291	0.031600	-0.355770
H	-3.708166	-1.733557	-0.448729
O	-1.535716	-1.894799	-1.512894
H	-1.316525	-2.780701	-1.207789
C	2.603076	-1.374638	0.561148
C	3.754367	-0.618920	0.609698
C	3.723296	0.703448	0.181616
C	2.555215	1.271701	-0.292941
H	2.584417	-2.400495	0.894987
H	4.671370	-1.047613	0.982030
H	4.623477	1.297896	0.223923
H	2.511194	2.299437	-0.614638

TS-H4-7

C	0.312960	1.132632	-1.043381
C	-0.950967	0.722855	-1.272619
C	-1.469017	-0.526843	-0.682309
C	-0.393693	-1.577439	-0.401928
C	0.951439	-1.114804	-0.110088
C	1.290987	0.202895	-0.428093
O	0.747287	2.335725	-1.283280
O	-0.736031	-2.740443	-0.423943
H	-1.666810	1.386416	-1.732914
H	0.183210	3.041840	-0.536524
N	-2.079675	-0.142740	0.657439
H	-2.910617	0.368305	0.377491
H	-1.464834	0.661883	1.223206
O	-0.374052	3.555805	0.412182
H	-1.059553	4.177879	0.188277
H	-0.717004	2.663222	1.176653
O	-0.987277	1.749161	1.851210
H	-0.332177	1.649599	2.536656
C	-2.490103	-1.241883	1.533922
H	-3.088461	-0.834290	2.341203
H	-1.612162	-1.720445	1.951934
H	-3.068176	-1.975741	0.981742
O	-2.479512	-1.105191	-1.420029
H	-2.367267	-2.060556	-1.352688
C	1.888646	-1.990293	0.424147
C	3.171008	-1.547204	0.673983
C	3.512206	-0.235554	0.369385
C	2.584994	0.632369	-0.180453
H	1.589796	-3.005174	0.636968
H	3.903847	-2.214615	1.099311
H	4.516938	0.111234	0.558377
H	2.836919	1.648765	-0.436272

TS-H4-8

C	-0.578489	-0.983282	-1.174441
C	0.753714	-1.110279	-1.317617
C	1.678634	-0.184420	-0.630747
C	1.107372	1.215190	-0.417184
C	-0.322283	1.317863	-0.180070
C	-1.136801	0.241269	-0.542986
O	-1.439521	-1.903526	-1.510790
O	1.884123	2.145446	-0.420663
H	1.176145	-1.992614	-1.772444
H	-1.660102	-2.458666	-0.505618
N	1.890962	-0.766351	0.758692
H	2.338317	-1.657360	0.571040
H	0.894317	-1.063734	1.277278
O	-1.748156	-2.837542	0.655092
H	-1.700834	-3.784008	0.754431
H	-0.926029	-2.225756	1.341949
O	-0.163126	-1.578056	1.932668
H	-0.651129	-0.979099	2.492396
C	2.743978	0.007940	1.662767
H	2.952045	-0.593727	2.540557
H	2.225439	0.909473	1.968203
H	3.673507	0.275465	1.171614
O	2.913437	-0.091944	-1.227977
H	3.185953	0.831578	-1.168408
C	-0.860578	2.481617	0.353454
C	-2.221413	2.567976	0.566767
C	-3.035175	1.496989	0.221964
C	-2.502621	0.346874	-0.334720
H	-0.197242	3.297517	0.596605
H	-2.649612	3.461315	0.993398
H	-4.100546	1.563538	0.382899
H	-3.129055	-0.480907	-0.624503

TS-H4-9

C	0.103098	1.212692	-0.933267
C	-1.037242	0.545581	-1.202885
C	-1.265450	-0.815486	-0.689928
C	0.013183	-1.603093	-0.387842
C	1.228645	-0.866503	-0.094698
C	1.271102	0.502132	-0.369406
O	0.247693	2.496248	-1.099650
O	-0.071163	-2.813283	-0.413664
H	-1.886195	1.069009	-1.615340
H	-0.637441	2.978596	-0.567632
N	-2.031166	-0.648646	0.623934
H	-2.948035	-0.362210	0.295371
H	-1.678771	0.242888	1.203194
O	-1.589675	3.269697	0.204312
H	-1.521215	4.166173	0.519927
H	-1.505009	2.404924	1.100959
O	-1.386417	1.489974	1.791195
H	-1.519292	1.703018	2.709594
C	-2.185111	-1.840454	1.461408
H	-2.924158	-1.633415	2.227620
H	-1.238812	-2.075514	1.933325
H	-2.505659	-2.684932	0.860822
O	-2.076771	-1.583769	-1.497680
H	-1.760682	-2.492394	-1.433797
C	2.341768	-1.534004	0.402069
C	3.502931	-0.832724	0.651567
C	3.547531	0.530466	0.388596
C	2.444644	1.194218	-0.118435
H	2.271565	-2.594885	0.586503
H	4.369666	-1.338955	1.046361
H	4.456702	1.080342	0.579608
H	2.465579	2.249994	-0.333232

TS-P1-1

C	-0.682986	-0.298899	-0.310097
C	0.793418	-0.589257	-0.242410
C	1.727027	0.435548	-0.150669
C	1.307523	1.850697	-0.262932
C	-0.095183	2.100107	-0.620788
C	-0.998725	1.127454	-0.656955
O	-1.316390	-1.197156	-1.084799
O	2.087871	2.763435	-0.098992
N	-1.238431	-0.512240	1.122503
H	-0.345279	3.121780	-0.863023
H	-2.027918	1.307204	-0.937995
H	-1.224936	-1.520970	1.232747
C	-0.558134	0.142222	2.239802
H	-2.293350	-0.225733	1.121234
H	-2.335691	-0.891927	-1.283427
O	-3.585012	-0.378035	-1.337524
O	-3.741914	0.025513	1.004968
H	-3.830640	-0.156341	-0.092209
H	-4.167000	0.843219	1.246285
H	-4.228758	-0.905421	-1.800811
C	1.217408	-1.907928	-0.214495
C	2.562578	-2.199105	-0.078086
C	3.494332	-1.175788	0.031058
C	3.077345	0.138538	-0.013449
H	0.487409	-2.693762	-0.336327
H	2.888970	-3.227772	-0.067869
H	4.542865	-1.407708	0.134557
H	3.776155	0.958446	0.046420
H	-1.136391	-0.020356	3.142907
H	-0.503581	1.207369	2.042023
H	0.443107	-0.253937	2.362863

TS-P1-2

C	0.638972	-0.142537	0.324082
C	-0.829288	-0.480218	0.276300
C	-1.771574	0.500596	-0.015869
C	-1.379113	1.926866	-0.085672
C	-0.019065	2.256337	0.363028
C	0.894553	1.318067	0.585787
O	1.306997	-0.972897	1.136092
O	-2.151686	2.787562	-0.447311
N	1.184276	-0.334208	-1.124770
H	0.189450	3.305089	0.509396
H	1.894675	1.550776	0.926555
C	1.206202	-1.724523	-1.585748
H	0.639044	0.242343	-1.754787
H	2.214781	0.037213	-1.143452
H	2.308701	-0.618519	1.310206
O	3.541268	-0.040562	1.326969
O	3.655167	0.309772	-1.025165
H	3.758716	0.158935	0.081677
H	4.050097	1.134663	-1.292262
H	4.222138	-0.514317	1.795009
C	-1.241785	-1.785695	0.484121
C	-2.580930	-2.114125	0.367132
C	-3.516816	-1.142939	0.041266
C	-3.113452	0.164516	-0.139248
H	-0.505055	-2.523479	0.760545
H	-2.898494	-3.131187	0.539102
H	-4.559583	-1.404684	-0.048602
H	-3.818708	0.951749	-0.356292
H	1.827652	-1.783763	-2.472072
H	0.202636	-2.071684	-1.802043
H	1.643821	-2.322743	-0.795348

TS-P1-3

C	-0.683098	-0.290032	-0.305507
C	0.793483	-0.581029	-0.228857
C	1.733567	0.438540	-0.151484
C	1.323130	1.855321	-0.270958
C	-0.088568	2.114863	-0.580337
C	-0.997980	1.147720	-0.600757
O	-1.292699	-1.167433	-1.121094
O	2.115764	2.762942	-0.141290
N	-1.263150	-0.547021	1.110260
H	-0.344539	3.143048	-0.785661
H	-2.038949	1.350561	-0.808931
H	-1.252118	-1.558523	1.189667
C	-0.594888	0.078956	2.251569
H	-2.311838	-0.238228	1.098393
H	-2.338240	-0.926549	-1.290450
O	-3.637712	-0.616216	-1.279728
O	-3.679436	0.303348	0.907312
H	-3.820062	-0.082871	-0.139134
H	-4.414016	0.047889	1.457763
H	-4.018996	-0.201431	-2.046913
C	1.211513	-1.901953	-0.195285
C	2.555030	-2.200162	-0.061706
C	3.493259	-1.181205	0.034374
C	3.083229	0.134589	-0.019957
H	0.477779	-2.685200	-0.312381
H	2.875402	-3.230635	-0.044965
H	4.540976	-1.418086	0.134877
H	3.786619	0.951336	0.028185
H	-1.174338	-0.115676	3.147385
H	-0.554837	1.149870	2.086068
H	0.409816	-0.311129	2.366117

TS-P1-4

C	-0.635714	-0.135544	-0.320020
C	0.830240	-0.483731	-0.253694
C	1.785510	0.492154	0.011042
C	1.413022	1.924554	0.050027
C	0.045344	2.261260	-0.365398
C	-0.880658	1.329770	-0.561009
O	-1.284834	-0.957316	-1.154205
O	2.205459	2.783698	0.369958
N	-1.211857	-0.335148	1.118346
H	-0.164388	3.311683	-0.496134
H	-1.893242	1.582630	-0.841029
C	-1.297024	-1.732427	1.546892
H	-0.650739	0.205945	1.765783
H	-2.220913	0.092238	1.131288
H	-2.320684	-0.678885	-1.287037
O	-3.616398	-0.323008	-1.227467
O	-3.566296	0.661801	0.929640
H	-3.745616	0.245470	-0.105963
H	-4.302195	0.473614	1.504589
H	-4.016955	0.088398	-1.986734
C	1.228997	-1.798388	-0.434000
C	2.563891	-2.140254	-0.310899
C	3.511919	-1.172646	-0.010217
C	3.123870	0.143125	0.138328
H	0.484450	-2.533171	-0.697207
H	2.868807	-3.164764	-0.460082
H	4.551804	-1.444220	0.083883
H	3.838279	0.927799	0.333515
H	-1.900102	-1.783993	2.446896
H	-0.308995	-2.134227	1.738427
H	-1.776342	-2.291126	0.751658

TS-P1-5

C	-0.683412	-0.305386	-0.294543
C	0.795232	-0.588181	-0.233891
C	1.725836	0.439600	-0.150360
C	1.299754	1.853645	-0.256183
C	-0.109589	2.098859	-0.585128
C	-1.011537	1.124463	-0.614200
O	-1.308509	-1.200177	-1.081639
O	2.081833	2.767377	-0.106105
N	-1.233783	-0.550934	1.135739
H	-0.370997	3.122362	-0.806291
H	-2.047364	1.311104	-0.863603
H	-1.161804	-1.557050	1.243602
C	-0.593043	0.141572	2.253798
H	-2.299641	-0.312062	1.125067
H	-2.317391	-0.891346	-1.301906
O	-3.562805	-0.357847	-1.376258
O	-3.696532	0.136962	0.944808
H	-3.812455	-0.105567	-0.142759
H	-4.438728	-0.172999	1.454474
H	-4.219694	-0.825074	-1.882244
C	1.225226	-1.905372	-0.211602
C	2.572382	-2.191962	-0.086917
C	3.501104	-1.165120	0.014679
C	3.078406	0.147449	-0.025596
H	0.498180	-2.694570	-0.330607
H	2.902664	-3.219438	-0.080891
H	4.551416	-1.393000	0.108849
H	3.774186	0.970331	0.028464
H	-1.138582	-0.083129	3.163765
H	-0.637657	1.209566	2.073378
H	0.440299	-0.170505	2.353751

TS-P1-6

C	-0.511482	-0.764219	0.505128
C	0.234862	-2.045560	0.743605
C	1.513297	-2.221466	0.435490
C	2.331580	-1.128328	-0.109250
C	1.743934	0.227696	-0.054955
C	0.415562	0.421211	0.318869
O	-1.452697	-0.635257	1.455183
O	3.447035	-1.333704	-0.535576
N	-1.199889	-0.930035	-0.869060
H	-0.361605	-2.836130	1.175332
H	2.017213	-3.164109	0.584136
C	-2.193924	-2.008479	-0.919860
H	-0.480290	-1.080105	-1.566738
H	-1.734406	-0.009751	-1.156942
H	-2.177441	0.116321	1.264596
O	-3.116578	1.058183	0.859588
O	-2.738540	0.996196	-1.485432
H	-3.048394	1.120369	-0.416238
H	-2.478730	1.835595	-1.854629
H	-3.987369	0.987999	1.238696
C	-0.069231	1.710535	0.472799
C	0.763477	2.790703	0.236564
C	2.078691	2.599153	-0.160194
C	2.569554	1.317622	-0.298965
H	-1.090199	1.867589	0.789098
H	0.381947	3.791452	0.370336
H	2.719647	3.447640	-0.342640
H	3.594264	1.128045	-0.578481
H	-2.756671	-1.910270	-1.840816
H	-1.711761	-2.978655	-0.873804
H	-2.858658	-1.882302	-0.073979

TS-P1-7

C	-0.480159	-0.901264	0.540307
C	0.469980	-2.023325	0.837591
C	1.779312	-1.968332	0.635241
C	2.421330	-0.753258	0.116371
C	1.589686	0.468911	0.065965
C	0.222189	0.424180	0.330601
O	-1.448821	-0.924762	1.471243
O	3.586234	-0.755459	-0.218121
N	-1.146136	-1.266875	-0.807187
H	-0.010194	-2.908025	1.233372
H	2.431925	-2.802274	0.843430
H	-1.626633	-2.142201	-0.626692
C	-0.300139	-1.378670	-1.996779
H	-1.950561	-0.553547	-1.040455
H	-2.294236	-0.267675	1.317627
O	-3.360911	0.505443	1.008439
O	-3.158089	0.211413	-1.343439
H	-3.407917	0.407236	-0.277265
H	-3.124307	1.031360	-1.828232
H	-4.159688	0.284309	1.478068
C	-0.501395	1.606112	0.368942
C	0.133679	2.811767	0.124116
C	1.489473	2.853469	-0.164164
C	2.217361	1.682024	-0.185225
H	-1.552368	1.587972	0.617314
H	-0.436144	3.727309	0.168813
H	1.975901	3.797760	-0.353327
H	3.278439	1.675303	-0.380392
H	-0.924531	-1.661960	-2.836945
H	0.148366	-0.412792	-2.197859
H	0.479694	-2.117412	-1.849928

TS-P2-1

C	-0.093709	1.209925	-0.618130
C	0.948699	0.434128	-0.966496
C	0.952053	-1.024899	-0.755770
C	-0.265940	-1.589625	-0.044923
C	-1.481260	-0.786568	-0.040223
C	-1.387188	0.587514	-0.284379
O	-0.029451	2.510123	-0.537671
O	-0.165343	-2.674460	0.492594
H	1.001986	2.718458	-0.140965
N	2.131525	-1.408602	0.070450
H	1.875988	-2.265357	0.558903
H	2.317132	-0.583560	0.791786
O	2.175552	2.671938	0.386749
H	2.475331	3.490555	0.769412
H	2.483040	1.581812	1.036894
O	2.716932	0.603027	1.516014
H	2.491434	0.662828	2.440371
C	3.365251	-1.594154	-0.694963
H	4.171645	-1.831834	-0.011180
H	3.604042	-0.667329	-1.203550
H	3.240996	-2.392466	-1.419647
H	1.028684	-1.594550	-1.689635
H	1.869483	0.907810	-1.270491
C	-2.528273	1.366724	-0.167562
C	-3.738713	0.779642	0.151407
C	-3.828258	-0.586311	0.391710
C	-2.693413	-1.365996	0.314869
H	-2.437032	2.428948	-0.327413
H	-4.624210	1.392841	0.224517
H	-4.776893	-1.031210	0.647867
H	-2.719288	-2.424032	0.525251

TS-P2-2

C	-0.111254	1.204452	-0.638203
C	0.942140	0.433447	-0.964784
C	0.958347	-1.023846	-0.737293
C	-0.247138	-1.586136	-0.004357
C	-1.473418	-0.801123	-0.020405
C	-1.397330	0.568206	-0.295265
O	-0.067819	2.505643	-0.585571
O	-0.129050	-2.654741	0.561429
H	0.927933	2.749356	-0.085581
N	2.153675	-1.396158	0.068622
H	1.893643	-2.224927	0.601444
H	2.386726	-0.539352	0.746821
O	1.994918	2.777855	0.586836
H	2.636937	3.418425	0.297609
H	2.467365	1.663579	1.005441
O	2.838978	0.664212	1.373469
H	2.901434	0.705889	2.323903
C	3.354939	-1.648433	-0.727395
H	4.182073	-1.864455	-0.061280
H	3.591396	-0.755615	-1.294794
H	3.191127	-2.482242	-1.402681
H	1.017802	-1.601811	-1.667750
H	1.860127	0.907018	-1.277124
C	-2.548997	1.334158	-0.197510
C	-3.751963	0.737833	0.132170
C	-3.823443	-0.623509	0.403339
C	-2.677963	-1.389011	0.346654
H	-2.470294	2.394003	-0.378443
H	-4.645721	1.340528	0.190710
H	-4.766406	-1.075256	0.668340
H	-2.689610	-2.442023	0.582027

TS-P2-3

C	-0.101078	1.206765	-0.616756
C	0.953495	0.435739	-0.940135
C	0.957811	-1.023621	-0.729163
C	-0.254432	-1.587760	-0.008667
C	-1.475845	-0.794947	-0.020615
C	-1.391768	0.575803	-0.284994
O	-0.051822	2.507272	-0.560202
O	-0.146375	-2.665806	0.540617
H	0.975904	2.739313	-0.136900
N	2.147344	-1.419275	0.076455
H	1.877553	-2.254645	0.594223
H	2.373853	-0.581849	0.764196
O	2.118975	2.765115	0.421082
H	2.203454	3.531303	0.981347
H	2.443387	1.659929	1.003319
O	2.706491	0.653701	1.434069
H	3.383758	0.740685	2.098026
C	3.350130	-1.661801	-0.719887
H	4.169157	-1.918990	-0.057930
H	3.603648	-0.752302	-1.252615
H	3.177878	-2.468341	-1.425196
H	1.017923	-1.590771	-1.666224
H	1.874248	0.909645	-1.245252
C	-2.540681	1.346179	-0.189405
C	-3.748141	0.753423	0.130230
C	-3.827253	-0.609201	0.392130
C	-2.685060	-1.379702	0.335514
H	-2.457329	2.406535	-0.365097
H	-4.639545	1.359751	0.187300
H	-4.773650	-1.058406	0.649084
H	-2.702867	-2.434456	0.562497

TS-P2-4

C	0.044459	1.246113	-0.865229
C	1.041088	0.466022	-1.328044
C	1.121541	-0.973056	-1.008363
C	-0.170463	-1.619572	-0.529255
C	-1.290937	-0.751140	-0.168525
C	-1.183245	0.632725	-0.325193
O	0.108601	2.548178	-0.822249
O	-0.221383	-2.828059	-0.457272
H	1.118412	2.768747	-0.348969
N	2.173001	-1.102596	0.067841
H	3.026519	-0.767598	-0.364486
H	2.003603	-0.316319	0.861605
O	2.201630	2.722414	0.309078
H	2.454439	3.553833	0.698944
H	2.133075	1.738912	1.120672
O	2.041569	0.786757	1.726685
H	1.337308	0.891520	2.361154
C	2.428599	-2.429488	0.639727
H	3.311618	-2.360344	1.265372
H	2.576814	-3.161459	-0.146820
H	1.583574	-2.737006	1.240483
H	1.466557	-1.589670	-1.838777
H	1.920754	0.941962	-1.736754
C	-2.252779	1.435642	0.041929
C	-3.410975	0.865473	0.537949
C	-3.517454	-0.511359	0.687221
C	-2.455151	-1.318332	0.335423
H	-2.149371	2.502182	-0.075398
H	-4.240965	1.498756	0.812776
H	-4.424020	-0.946811	1.077356
H	-2.500747	-2.391044	0.442195

TS-P2-5

C	0.002313	1.228958	0.910913
C	-1.018802	0.469114	1.355615
C	-1.142082	-0.964592	1.020803
C	0.123780	-1.638560	0.508990
C	1.263027	-0.797987	0.146876
C	1.200236	0.584237	0.335493
O	-0.003229	2.531003	0.922623
O	0.137497	-2.847107	0.418157
H	-0.926896	2.846361	0.296123
N	-2.224759	-1.066293	-0.025216
H	-3.067557	-0.761175	0.446868
H	-2.100082	-0.243141	-0.807717
O	-1.839129	2.957119	-0.522954
H	-2.606369	3.433880	-0.222565
H	-2.066622	1.880651	-1.108218
O	-2.208870	0.860021	-1.619553
H	-1.795445	0.878899	-2.478270
C	-2.489321	-2.374100	-0.635762
H	-3.395843	-2.290453	-1.225395
H	-2.600371	-3.138361	0.125717
H	-1.664857	-2.650248	-1.279109
H	-1.476085	-1.580292	1.856844
H	-1.869816	0.956775	1.809447
C	2.288917	1.361776	-0.029371
C	3.420356	0.767981	-0.557852
C	3.481918	-0.607860	-0.739616
C	2.401187	-1.389689	-0.388029
H	2.218598	2.427845	0.113725
H	4.264757	1.381825	-0.832932
H	4.368279	-1.061729	-1.154495
H	2.412309	-2.460739	-0.518048

TS-O1-1

C	0.575970	-0.627144	-0.209341
C	0.291210	-2.132108	-0.117207
C	-1.035164	-2.575253	-0.502152
C	-2.046401	-1.701031	-0.493316
C	-1.893550	-0.301210	-0.137094
C	-0.625219	0.237475	0.097055
O	1.034136	-0.475288	-1.471965
H	-3.047742	-2.038400	-0.722513
N	1.712377	-0.369453	0.743868
O	1.187537	-2.882171	0.200386
H	-1.171860	-3.624296	-0.708753
H	2.382746	-1.087053	0.474401
C	1.419412	-0.504120	2.173561
H	2.170723	0.597182	0.541817
H	1.255496	0.576691	-1.736350
O	1.685205	1.792448	-1.912748
H	1.028662	2.425633	-2.187517
O	2.659451	1.984016	0.243304
H	2.244623	2.026494	-0.824843
H	3.588746	2.195372	0.247312
C	-0.506182	1.562572	0.476220
C	-1.637027	2.352024	0.626167
C	-2.893404	1.827180	0.382354
C	-3.017349	0.504441	0.001203
H	0.468534	1.995827	0.648589
H	-1.528798	3.382328	0.927795
H	-3.772087	2.443561	0.490605
H	-3.993796	0.082330	-0.186354
H	2.333050	-0.334376	2.731831
H	1.047240	-1.500937	2.381265
H	0.683415	0.236830	2.459112

TS-O1-2

C	-0.556468	0.638917	-0.214116
C	-0.232931	2.138737	-0.150819
C	1.107541	2.546760	-0.518106
C	2.097944	1.648556	-0.485390
C	1.906963	0.253870	-0.132004
C	0.623532	-0.255007	0.083965
O	-1.053914	0.470420	-1.460691
H	3.110660	1.961933	-0.698546
N	-1.678735	0.435371	0.770864
O	-1.117046	2.913392	0.144351
H	1.272868	3.590947	-0.728256
H	-2.318528	1.186713	0.517860
C	-1.338766	0.557411	2.190654
H	-2.189118	-0.504084	0.580136
H	-1.270346	-0.578573	-1.695913
O	-1.635325	-1.845881	-1.805153
H	-2.058978	-2.062185	-2.630387
O	-2.765355	-1.861189	0.282878
H	-2.341028	-1.968140	-0.770497
H	-3.702695	-2.029825	0.300240
C	0.464419	-1.582862	0.434677
C	1.572691	-2.402251	0.586421
C	2.845251	-1.904810	0.371927
C	3.008683	-0.580838	0.010534
H	-0.522615	-1.997950	0.574626
H	1.433177	-3.436386	0.859829
H	3.706138	-2.545625	0.481521
H	3.997689	-0.181944	-0.161534
H	-2.245666	0.452680	2.775285
H	-0.895504	1.528611	2.381346
H	-0.644943	-0.228609	2.460700

TS-O1-3

C	-0.528328	0.643566	-0.215758
C	-0.164484	2.135105	-0.169071
C	1.188053	2.507696	-0.532303
C	2.157662	1.588114	-0.485529
C	1.929998	0.198550	-0.132851
C	0.632989	-0.278227	0.071226
O	-1.049448	0.472201	-1.450772
H	3.179025	1.876832	-0.691970
N	-1.634775	0.477843	0.794353
O	-1.027098	2.935135	0.119696
H	1.378814	3.546414	-0.748100
H	-2.275219	1.227323	0.537253
C	-1.264341	0.627309	2.203440
H	-2.171026	-0.452464	0.642549
H	-1.328961	-0.566399	-1.664148
O	-1.783722	-1.809336	-1.771490
H	-2.261191	-1.946746	-2.584951
O	-2.975918	-1.657104	0.273253
H	-2.506126	-1.853966	-0.748447
H	-3.148904	-2.454276	0.763737
C	0.437708	-1.606778	0.398876
C	1.520878	-2.458412	0.548914
C	2.807903	-1.990128	0.353779
C	3.008176	-0.667008	0.008669
H	-0.565067	-1.990332	0.510980
H	1.353439	-3.493213	0.803746
H	3.651101	-2.654153	0.462329
H	4.008524	-0.293283	-0.153874
H	-2.158956	0.533976	2.808737
H	-0.817811	1.601743	2.367152
H	-0.562027	-0.152246	2.472698

TS-O1-4

C	-0.421936	-0.130116	-0.276365
C	1.089305	-0.225023	-0.281667
C	1.855072	0.836714	0.205287
C	1.205953	2.098421	0.528633
C	-0.070330	2.352167	0.215043
C	-0.866690	1.333939	-0.482769
O	-1.003304	-1.019769	-1.053151
N	-0.851735	-0.378512	1.203440
H	-0.519837	3.321860	0.360814
H	1.816699	2.871964	0.974082
O	-1.824778	1.610596	-1.155749
C	-0.538325	-1.733423	1.652838
H	-0.418983	0.309739	1.808600
H	-1.994240	-0.254091	1.253579
H	-2.213452	-0.913003	-1.168037
O	-3.385367	-0.819596	-1.142679
O	-3.337650	-0.138464	1.132021
H	-3.498433	-0.482520	-0.011916
H	-3.912701	-0.598037	1.737169
H	-3.594591	-0.069856	-1.697469
C	1.703662	-1.381633	-0.713813
C	3.083465	-1.505309	-0.636212
C	3.847381	-0.472024	-0.120591
C	3.235074	0.698022	0.292856
H	1.081342	-2.163741	-1.120368
H	3.561938	-2.408864	-0.981462
H	4.919848	-0.569977	-0.055765
H	3.828972	1.519415	0.666704
H	-1.069495	-1.930197	2.578487
H	0.528182	-1.858881	1.805426
H	-0.880083	-2.416774	0.883107

TS-O1-5

C	-0.411413	-0.114992	-0.282866
C	1.098129	-0.226329	-0.275423
C	1.877058	0.838921	0.181122
C	1.245540	2.117487	0.462249
C	-0.031814	2.377312	0.155431
C	-0.860433	1.349209	-0.482179
O	-0.989636	-1.000095	-1.066927
N	-0.862725	-0.352606	1.190274
H	-0.463403	3.359078	0.273596
H	1.869719	2.899242	0.873622
O	-1.873497	1.614470	-1.078971
C	-0.605666	-1.719063	1.645005
H	-0.408369	0.315674	1.802052
H	-2.015214	-0.192357	1.229571
H	-2.207361	-0.939554	-1.158947
O	-3.377996	-0.903018	-1.122220
O	-3.348568	-0.221404	1.157060
H	-3.498352	-0.541731	0.010083
H	-3.812021	0.587995	1.355095
H	-3.628838	-0.187806	-1.703890
C	1.700048	-1.403348	-0.669158
C	3.077710	-1.541989	-0.582383
C	3.854156	-0.502865	-0.097568
C	3.255549	0.686812	0.276455
H	1.070079	-2.189775	-1.054893
H	3.545218	-2.462368	-0.896873
H	4.925065	-0.612520	-0.026614
H	3.858287	1.512569	0.625770
H	-1.166567	-1.893969	2.556666
H	0.453168	-1.881945	1.816909
H	-0.957942	-2.390836	0.870285

TS-O1-6

C	-0.660582	0.360342	-0.411804
C	-0.834805	1.886068	-0.550788
C	0.142374	2.718836	0.153114
C	1.325788	2.214071	0.521740
C	1.721191	0.845259	0.240776
C	0.793931	-0.051605	-0.298165
O	-1.396465	-0.277880	-1.312014
H	2.059600	2.852497	0.994702
N	-1.235320	0.105357	1.009278
O	-1.789111	2.346828	-1.119004
H	-0.105407	3.760718	0.281976
C	-2.658128	0.448944	1.140859
H	-0.676865	0.612751	1.687290
H	-1.129150	-0.964020	1.241876
H	-1.488802	-1.341431	-1.168764
O	-1.592869	-2.661416	-0.866213
H	-2.373661	-3.088804	-1.205655
O	-1.262839	-2.401072	1.480691
H	-1.457781	-2.668854	0.418229
H	-0.520990	-2.902436	1.807514
C	1.199121	-1.318271	-0.673003
C	2.520096	-1.702875	-0.491923
C	3.437302	-0.830358	0.067465
C	3.038227	0.442784	0.429070
H	0.483463	-2.004990	-1.100466
H	2.829672	-2.692037	-0.792027
H	4.462170	-1.135734	0.209963
H	3.751299	1.141087	0.842419
H	-3.063048	-0.088962	1.990209
H	-3.152478	0.134402	0.228917
H	-2.787601	1.517458	1.267141

TS-O1-7

C	-0.398514	-0.102128	-0.163553
C	1.107376	-0.274859	-0.116427
C	1.926133	0.850151	-0.006678
C	1.337532	2.163566	0.185201
C	0.030595	2.356098	0.382142
C	-0.861968	1.211670	0.484693
O	-0.779435	-0.109934	-1.456340
N	-1.107199	-1.207366	0.555799
H	-0.392760	3.329992	0.568965
H	2.012531	3.008309	0.186345
O	-1.954205	1.289113	1.005281
H	-0.922124	-2.040430	0.011213
C	-0.753508	-1.414164	1.957032
H	-2.336739	-1.041534	0.446668
H	-1.953270	0.086876	-1.683047
O	-3.120475	0.186650	-1.817881
O	-3.559956	-0.923705	0.243615
H	-3.502392	-0.434032	-0.762403
H	-3.852278	-0.235874	0.841738
H	-3.412258	-0.168488	-2.652806
C	1.690670	-1.510481	-0.325718
C	3.067372	-1.646986	-0.397698
C	3.880396	-0.533320	-0.279025
C	3.306974	0.709268	-0.091033
H	1.074298	-2.388489	-0.453655
H	3.502232	-2.621791	-0.555471
H	4.952824	-0.632356	-0.339364
H	3.930730	1.587402	-0.008481
H	-1.320122	-2.254861	2.344148
H	-1.025360	-0.526682	2.517932
H	0.309304	-1.606361	2.076602

TS-O1-8

C	0.403394	-0.103136	0.175661
C	-1.103659	-0.280380	0.123272
C	-1.948460	0.826508	0.048832
C	-1.389176	2.160555	-0.051979
C	-0.078478	2.400242	-0.158819
C	0.860256	1.296927	-0.270042
O	0.811952	-0.313765	1.437250
N	1.087456	-1.076379	-0.736688
H	0.321960	3.396707	-0.258384
H	-2.086730	2.986986	-0.043427
O	2.002428	1.468174	-0.649010
H	0.897390	-1.989221	-0.342376
C	0.692126	-1.031288	-2.139861
H	2.369395	-0.944267	-0.632992
H	2.048767	-0.276589	1.687971
O	3.172070	-0.352790	1.835195
O	3.552696	-0.856448	-0.466425
H	3.529205	-0.608823	0.624672
H	3.781028	-0.036620	-0.906200
H	3.517528	0.450669	2.214333
C	-1.659517	-1.537172	0.279565
C	-3.032606	-1.709463	0.320277
C	-3.872772	-0.612319	0.225314
C	-3.328144	0.649877	0.099979
H	-1.018744	-2.398545	0.399545
H	-3.445776	-2.699289	0.438176
H	-4.943203	-0.740655	0.260803
H	-3.971664	1.515883	0.044398
H	1.228929	-1.799602	-2.687137
H	0.966634	-0.064129	-2.549317
H	-0.377868	-1.181335	-2.262515

TS-O1-9

C	-0.423416	-0.202242	-0.255219
C	1.083784	-0.367905	-0.209025
C	1.941504	0.727301	-0.114433
C	1.401720	2.072121	-0.188376
C	0.107443	2.329007	-0.406874
C	-0.862123	1.249627	-0.556639
O	-0.987572	-1.112087	-1.032587
N	-0.924624	-0.446943	1.186906
H	-0.268583	3.334094	-0.519176
H	2.103801	2.890420	-0.102184
O	-2.007932	1.464366	-0.875725
H	-0.592041	-1.384339	1.383490
C	-0.504092	0.466046	2.246648
H	-2.110215	-0.527678	1.173375
H	-2.229940	-1.055577	-1.209161
O	-3.374324	-1.040872	-1.238871
O	-3.409490	-0.592871	1.091761
H	-3.528872	-0.823628	-0.073617
H	-3.844724	-1.253245	1.624796
H	-3.606147	-0.242244	-1.710376
C	1.608272	-1.646607	-0.244090
C	2.975790	-1.846692	-0.147154
C	3.830576	-0.762765	-0.025285
C	3.314339	0.518659	-0.019201
H	0.928240	-2.473473	-0.385285
H	3.375826	-2.848436	-0.180092
H	4.896000	-0.916148	0.047157
H	3.975252	1.370718	0.047029
H	-0.824099	0.067265	3.203793
H	-0.984999	1.426845	2.099886
H	0.574632	0.596431	2.253289

TS-O1-10

C	-0.665641	0.346715	-0.402414
C	-0.853821	1.869711	-0.563500
C	0.119563	2.723024	0.116713
C	1.309933	2.233484	0.484630
C	1.713783	0.863610	0.227571
C	0.791796	-0.053265	-0.288230
O	-1.408968	-0.304251	-1.287368
H	2.042589	2.886139	0.939749
N	-1.238653	0.109091	1.027643
O	-1.818534	2.310280	-1.131385
H	-0.135238	3.765334	0.226789
C	-2.646930	0.501594	1.164464
H	-0.655803	0.594152	1.701411
H	-1.166964	-0.960394	1.254458
H	-1.464473	-1.369602	-1.168434
O	-1.534959	-2.706741	-0.901105
H	-2.309199	-3.140047	-1.247191
O	-1.130905	-2.417964	1.426058
H	-1.381966	-2.709280	0.377429
H	-1.638289	-2.913024	2.061727
C	1.207154	-1.324523	-0.632387
C	2.532534	-1.691858	-0.448468
C	3.444850	-0.798603	0.083553
C	3.035451	0.478653	0.417898
H	0.499511	-2.034067	-1.033830
H	2.846556	-2.687699	-0.719568
H	4.472669	-1.092021	0.229825
H	3.742964	1.193155	0.812785
H	-3.073298	-0.020408	2.013852
H	-3.153560	0.209408	0.251302
H	-2.740031	1.572871	1.297621

TS-O1-11

C	0.400976	-0.084333	0.306291
C	-1.102823	-0.237011	0.266927
C	-1.904727	0.825392	-0.154917
C	-1.308164	2.132833	-0.372197
C	-0.040234	2.413854	-0.048454
C	0.828173	1.382676	0.528561
O	0.978019	-0.971076	1.095318
N	0.895503	-0.283001	-1.158032
H	0.365583	3.410512	-0.126661
H	-1.952699	2.913799	-0.752405
O	1.871992	1.640339	1.068464
C	0.703270	-1.647512	-1.647399
H	0.425505	0.378455	-1.765856
H	2.036893	-0.062865	-1.177103
H	2.155986	-0.967416	1.140934
O	3.365328	-1.014548	1.035909
O	3.379431	-0.010790	-1.116136
H	3.508137	-0.510191	-0.069293
H	3.740216	0.871779	-1.067972
H	3.708256	-1.900999	1.106596
C	-1.679455	-1.445201	0.602069
C	-3.050882	-1.618028	0.487492
C	-3.848505	-0.580246	0.035451
C	-3.277117	0.639822	-0.277250
H	-1.036319	-2.230626	0.967070
H	-3.496920	-2.563423	0.755481
H	-4.914893	-0.715240	-0.056785
H	-3.897102	1.463865	-0.599232
H	1.282497	-1.777300	-2.555221
H	-0.345203	-1.851068	-1.838116
H	1.070316	-2.323149	-0.883101

TS-O1-12

C	0.647714	0.420616	0.412040
C	0.769475	1.958591	0.447100
C	-0.246914	2.713368	-0.285560
C	-1.417597	2.148950	-0.605939
C	-1.758064	0.784433	-0.249211
C	-0.791454	-0.046285	0.322546
O	1.385169	-0.122408	1.381647
H	-2.179477	2.735574	-1.101076
N	1.259045	0.075676	-0.965043
O	1.716163	2.487670	0.968499
H	-0.036826	3.754101	-0.475345
C	2.723263	0.228166	-1.008553
H	0.810993	0.659483	-1.663975
H	1.036696	-0.968838	-1.230303
H	1.618112	-1.121816	1.201779
O	1.976281	-2.411275	0.701032
H	2.079216	-3.147368	1.295261
O	0.905267	-2.422182	-1.412442
H	1.418961	-2.604242	-0.431061
H	1.369674	-2.864675	-2.117295
C	-1.139474	-1.310580	0.751233
C	-2.442715	-1.759705	0.603395
C	-3.401401	-0.949587	0.021169
C	-3.059461	0.320971	-0.402168
H	-0.385428	-1.946626	1.186876
H	-2.705110	-2.750744	0.939038
H	-4.413518	-1.303685	-0.097332
H	-3.804287	0.969193	-0.840307
H	3.045977	0.099972	-2.036153
H	3.150482	-0.549257	-0.386886
H	3.017950	1.201112	-0.634110

TS-O1-13

C	-0.416507	-0.115950	-0.288116
C	1.090624	-0.240963	-0.274788
C	1.868002	0.825956	0.182214
C	1.237237	2.109790	0.455681
C	-0.030239	2.373084	0.117827
C	-0.837570	1.343571	-0.556415
O	-1.004976	-1.027538	-1.038158
N	-0.861918	-0.298413	1.198606
H	-0.466344	3.353714	0.226346
H	1.857089	2.886704	0.882205
O	-1.779661	1.602843	-1.251033
C	-0.596411	-1.643858	1.704111
H	-0.403890	0.399042	1.774367
H	-1.974275	-0.121686	1.246442
H	-2.170390	-0.942185	-1.135676
O	-3.394539	-0.902991	-1.074939
O	-3.344727	0.054657	1.093949
H	-3.524504	-0.427888	0.030563
H	-4.002722	-0.171280	1.743529
H	-3.775252	-1.772962	-1.157995
C	1.690665	-1.421871	-0.659613
C	3.067254	-1.564901	-0.563547
C	3.842037	-0.525853	-0.076759
C	3.244469	0.667509	0.288793
H	1.061316	-2.208832	-1.045065
H	3.534435	-2.487520	-0.871768
H	4.912161	-0.637936	0.002608
H	3.848006	1.492158	0.639207
H	-1.134148	-1.783423	2.636016
H	0.465538	-1.797265	1.861436
H	-0.959740	-2.346595	0.962660

TS-O1-14

C	-0.394964	-0.113910	-0.166714
C	1.109956	-0.275847	-0.127970
C	1.898464	0.865287	0.037236
C	1.278379	2.151042	0.314246
C	-0.023579	2.287444	0.572683
C	-0.868798	1.100825	0.643880
O	-0.765474	0.021641	-1.461898
N	-1.101153	-1.316169	0.391982
H	-0.472530	3.231090	0.837190
H	1.929230	3.013856	0.340157
O	-1.901814	1.064176	1.264899
H	-0.860389	-2.069832	-0.240229
C	-0.812623	-1.687551	1.778077
H	-2.234239	-1.186144	0.238796
H	-1.811849	0.408811	-1.573552
O	-3.045339	0.759618	-1.536615
O	-3.566420	-1.024540	-0.049422
H	-3.475870	-0.161113	-0.785501
H	-4.012718	-1.755966	-0.468119
H	-3.468464	0.852442	-2.384646
C	1.723095	-1.484521	-0.397941
C	3.103207	-1.581288	-0.482423
C	3.885365	-0.453223	-0.314973
C	3.280578	0.763547	-0.061764
H	1.134143	-2.375570	-0.561105
H	3.562330	-2.535884	-0.687140
H	4.959669	-0.520082	-0.385271
H	3.882491	1.651634	0.063577
H	-1.326529	-2.615463	2.004554
H	-1.194290	-0.909097	2.425902
H	0.254967	-1.813506	1.929770

TS-O2-1

C	-0.176199	-1.162441	0.643050
C	1.013157	-0.366005	1.041005
C	1.017461	1.143730	0.866675
C	-0.241583	1.752607	0.395453
C	-1.346926	0.991084	0.204304
C	-1.329066	-0.460021	0.305985
O	-0.037138	-2.419925	0.569095
H	-0.308695	2.828685	0.344034
H	1.120963	-2.641533	-0.244761
N	2.165183	1.350209	-0.055673
H	2.968169	0.956447	0.423705
H	1.952731	0.497474	-1.070414
O	1.923365	-2.572417	-0.914133
H	2.707509	-2.654062	-0.371186
H	1.866124	-1.443116	-1.402698
O	1.769223	-0.355704	-1.822480
H	0.935530	-0.245147	-2.279118
C	2.427163	2.734628	-0.417369
H	3.335399	2.778354	-1.009565
H	2.544480	3.364571	0.463392
H	1.604935	3.113434	-1.013832
H	1.285518	1.563994	1.842636
O	2.057796	-0.891692	1.377274
C	-2.505311	-1.199914	-0.019041
C	-3.653159	-0.582231	-0.368310
C	-3.697860	0.848889	-0.423262
C	-2.610835	1.594081	-0.150280
H	-2.433421	-2.274548	0.042957
H	-4.539877	-1.152099	-0.596556
H	-4.624803	1.335406	-0.688771
H	-2.657882	2.672145	-0.197412

TS-O2-2

C	-0.166761	1.007411	-0.568241
C	0.924426	0.068047	-0.958804
C	0.796602	-1.409591	-0.626987
C	-0.559264	-1.872755	-0.274123
C	-1.578248	-0.990785	-0.125375
C	-1.394464	0.448734	-0.234944
O	0.096965	2.246773	-0.571156
H	-0.733716	-2.936727	-0.203291
H	1.370520	2.495044	-0.056608
N	1.760493	-1.617944	0.506284
H	1.358905	-2.327516	1.104228
H	1.893780	-0.534979	1.188919
O	2.293031	2.503950	0.462438
H	2.962195	2.408948	-0.215159
H	2.247458	1.489600	1.129442
O	2.124817	0.494638	1.750484
H	1.553620	0.644704	2.501421
C	3.102207	-2.017198	0.080413
H	3.738371	-2.114606	0.954152
H	3.501494	-1.246395	-0.568132
H	3.075347	-2.960190	-0.461183
H	1.189107	-1.957230	-1.485981
O	1.965768	0.464304	-1.439518
C	-2.492257	1.320502	0.032910
C	-3.714497	0.840799	0.343370
C	-3.919554	-0.575873	0.409210
C	-2.914316	-1.442622	0.184876
H	-2.299200	2.379427	-0.039763
H	-4.539963	1.508640	0.531868
H	-4.904243	-0.952765	0.643738
H	-3.085008	-2.507675	0.240545

TS-O2-3

C	0.217631	-1.151372	-0.723062
C	-1.046593	-0.440215	-1.063883
C	-1.170477	1.059650	-0.844206
C	0.044060	1.743507	-0.351362
C	1.211527	1.068528	-0.204697
C	1.315208	-0.374380	-0.370058
O	0.168072	-2.417866	-0.681508
H	0.025871	2.817745	-0.246210
H	-0.888633	-2.676198	0.248125
N	-2.321113	1.159978	0.084478
H	-3.074294	0.643956	-0.358543
H	-1.888002	0.357896	1.159724
O	-1.539784	-2.615450	1.072615
H	-1.315582	-3.298518	1.700984
H	-1.488777	-1.477054	1.521054
O	-1.425814	-0.358649	1.867487
H	-0.509221	-0.098342	1.984520
C	-2.746546	2.515336	0.388429
H	-3.646335	2.476609	0.993874
H	-2.951247	3.088947	-0.515599
H	-1.973064	3.021120	0.956360
H	-1.463571	1.484129	-1.812074
O	-2.043588	-1.045682	-1.393443
C	2.553121	-1.026515	-0.085206
C	3.648712	-0.331407	0.284860
C	3.573284	1.094944	0.403431
C	2.425418	1.757803	0.170098
H	2.571943	-2.099366	-0.198209
H	4.582811	-0.833849	0.480144
H	4.458898	1.645898	0.683754
H	2.383834	2.833095	0.263469

TS-O2-4

C	-0.121327	0.965147	-0.652870
C	0.965556	0.010399	-1.032328
C	0.854693	-1.448591	-0.620309
C	-0.506063	-1.897821	-0.260771
C	-1.524250	-1.012655	-0.131435
C	-1.344155	0.424979	-0.284919
O	0.154868	2.204103	-0.697313
H	-0.680506	-2.958122	-0.146546
H	1.387618	2.423022	-0.144611
N	1.787546	-1.583968	0.545656
H	1.446158	-2.352814	1.106102
H	1.743808	-0.486154	1.278851
O	2.235837	2.427406	0.516719
H	2.294382	3.269467	0.962306
H	2.034478	1.483524	1.251220
O	1.755441	0.519365	1.871423
H	0.902565	0.648811	2.285755
C	3.183635	-1.817146	0.175232
H	3.780091	-1.894699	1.078670
H	3.535731	-0.979601	-0.415446
H	3.286341	-2.728717	-0.410097
H	1.268510	-2.039667	-1.439819
O	1.972933	0.395731	-1.577974
C	-2.440740	1.303791	-0.029698
C	-3.658342	0.832536	0.308933
C	-3.860926	-0.582828	0.416433
C	-2.857893	-1.455022	0.205202
H	-2.251900	2.360444	-0.139238
H	-4.483035	1.504428	0.486222
H	-4.842818	-0.953595	0.671557
H	-3.028031	-2.518119	0.291828

TS-O2-5

C	-0.288080	1.010787	-0.632062
C	0.877440	0.129918	-0.915411
C	0.823960	-1.345772	-0.560898
C	-0.478695	-1.853728	-0.087730
C	-1.555988	-1.034450	-0.009883
C	-1.478294	0.397340	-0.261563
O	-0.092557	2.260862	-0.711284
H	-0.581917	-2.916477	0.080196
H	1.115230	2.550330	-0.055850
N	1.922157	-1.551971	0.434387
H	1.557940	-2.161621	1.154241
H	2.298895	-0.410508	1.007585
O	1.903583	2.663702	0.641734
H	1.581398	3.239707	1.332344
H	2.298192	1.572864	1.082388
O	2.688489	0.570390	1.503648
H	3.643074	0.596159	1.465946
C	3.133867	-2.123471	-0.149456
H	3.879184	-2.266634	0.628014
H	3.514059	-1.427844	-0.889885
H	2.932426	-3.079904	-0.627722
H	1.117099	-1.873850	-1.472735
O	1.921811	0.577610	-1.338266
C	-2.635822	1.208664	-0.067397
C	-3.818585	0.675111	0.302553
C	-3.918681	-0.738560	0.513525
C	-2.853407	-1.547638	0.363953
H	-2.521009	2.266678	-0.244724
H	-4.690021	1.296921	0.433139
H	-4.871501	-1.160461	0.797768
H	-2.945048	-2.611283	0.528140

TS-O2-6

C	-1.526186	-0.366876	0.088942
C	-2.281472	0.764111	-0.301862
C	-3.688204	0.688270	-0.217676
C	-4.306934	-0.444515	0.226698
C	-3.548662	-1.564455	0.611006
C	-2.185294	-1.524053	0.541622
H	-4.271236	1.548185	-0.514159
H	-5.384300	-0.482903	0.283217
H	-4.048646	-2.455179	0.959624
H	-1.577170	-2.367230	0.828694
C	-0.102536	-0.341955	0.006549
C	0.479010	0.836012	-0.424600
C	-0.258516	1.958300	-0.809115
C	-1.622185	1.926031	-0.759527
H	0.274387	2.831716	-1.153319
O	0.623283	-1.368804	0.376876
O	1.863389	0.885895	-0.524614
H	-2.204243	2.782600	-1.062613
N	2.477488	0.604800	0.708143
O	2.404237	-2.110913	-1.047617
H	3.428066	-1.527558	-0.690833
H	3.500244	-0.026950	0.320789
H	1.534406	-1.781878	-0.423510
O	4.224230	-0.797172	-0.265448
H	4.877167	-1.233073	0.276456
H	1.881596	-0.102254	1.149402
C	2.602414	1.811408	1.501525
H	3.263100	2.501252	0.989100
H	3.028748	1.544893	2.464365
H	1.627901	2.268985	1.648602
H	2.437845	-3.059930	-1.127743

TS-O3-1

C	-0.909195	-0.216904	-0.216982
C	0.358250	-1.059250	-0.357183
C	1.643872	-0.374780	-0.200895
C	1.680797	0.853309	0.467476
C	0.450648	1.458743	0.961143
C	-0.752650	0.959666	0.698724
O	-1.243433	0.123892	-1.482628
C	2.913223	1.461900	0.664941
N	-1.980125	-1.130535	0.319321
O	0.253746	-2.232749	-0.631171
C	2.808248	-0.976318	-0.650732
H	0.546832	2.362752	1.545165
H	-1.658630	1.441069	1.039272
H	-2.030480	-1.876820	-0.368207
C	-1.752685	-1.677021	1.658711
H	-2.909308	-0.561833	0.326188
H	-2.020636	0.897182	-1.494895
O	-3.076773	1.678359	-1.365886
H	-2.918386	2.616139	-1.320546
O	-3.976692	0.472037	0.472900
H	-3.662095	1.143013	-0.385201
H	-4.901616	0.256771	0.393844
H	-2.611495	-2.273325	1.945054
H	-1.645649	-0.853775	2.355827
H	-0.860571	-2.292243	1.665263
C	4.025114	-0.349777	-0.463195
C	4.072458	0.869120	0.197261
H	2.734766	-1.930082	-1.149956
H	4.932719	-0.805771	-0.825896
H	5.021252	1.359855	0.351298
H	2.960907	2.406371	1.186211

TS-O3-2

C	0.913460	0.218356	-0.224495
C	-0.358804	1.052452	-0.377900
C	-1.643731	0.371728	-0.211742
C	-1.677918	-0.855928	0.457699
C	-0.445604	-1.469855	0.934527
C	0.757574	-0.972606	0.670401
O	1.287377	-0.109251	-1.483836
C	-2.910863	-1.460774	0.664650
N	1.959498	1.146371	0.338573
O	-0.253791	2.224630	-0.660255
C	-2.810299	0.976764	-0.652470
H	-0.538500	-2.387547	1.496930
H	1.663349	-1.478487	0.973796
H	1.984624	1.912463	-0.328621
C	1.712923	1.650857	1.690485
H	2.904263	0.609173	0.323932
H	2.021354	-0.913033	-1.459225
O	2.989001	-1.800604	-1.196857
H	3.451637	-2.142861	-1.955450
O	4.006834	-0.392859	0.429946
H	3.676618	-1.123198	-0.364388
H	4.931287	-0.182132	0.341434
H	2.546821	2.274985	1.990797
H	1.638503	0.807732	2.367564
H	0.796672	2.229817	1.711587
C	-4.027334	0.354617	-0.453928
C	-4.072104	-0.864237	0.207306
H	-2.737957	1.929961	-1.152968
H	-4.936773	0.813307	-0.808548
H	-5.020953	-1.352337	0.369436
H	-2.956593	-2.406030	1.184543

TS-O3-3

C	0.910219	0.195849	-0.212671
C	-0.357307	1.034697	-0.383615
C	-1.649197	0.365638	-0.219493
C	-1.698649	-0.859456	0.453454
C	-0.473803	-1.487954	0.929724
C	0.734464	-0.999315	0.672349
O	1.304515	-0.133364	-1.463830
C	-2.938107	-1.451397	0.658867
N	1.949500	1.118678	0.372075
O	-0.243616	2.203865	-0.673660
C	-2.808374	0.980611	-0.665972
H	-0.576907	-2.411627	1.480575
H	1.633092	-1.525325	0.961721
H	2.008911	1.875159	-0.304131
C	1.667808	1.648747	1.706792
H	2.897773	0.582946	0.387227
H	2.060470	-0.922641	-1.429945
O	3.052059	-1.779360	-1.181687
H	3.509288	-2.075463	-1.963416
O	4.112741	-0.261515	0.314076
H	3.750095	-1.049023	-0.403623
H	4.574544	-0.649088	1.051133
H	2.513468	2.242786	2.034584
H	1.525867	0.818591	2.390097
H	0.775979	2.264314	1.684530
C	-4.032283	0.371713	-0.468471
C	-4.091904	-0.844309	0.196754
H	-2.724927	1.931092	-1.169842
H	-4.935879	0.838588	-0.827311
H	-5.046214	-1.321985	0.357715
H	-2.994861	-2.395037	1.180648

TS-O3-4

C	0.831581	0.173655	0.003866
C	-0.380687	1.071517	0.236559
C	-1.690110	0.441524	0.040436
C	-1.799469	-0.934789	0.260076
C	-0.617225	-1.704143	0.629328
C	0.612242	-1.201651	0.573383
O	1.037251	0.152262	-1.338174
C	-3.053224	-1.521270	0.161839
N	2.010869	0.819426	0.701372
O	-0.237858	2.226910	0.561851
C	-2.802452	1.209449	-0.256776
H	-0.768900	-2.727660	0.939928
H	1.485611	-1.789106	0.815521
C	2.716787	1.821227	-0.118615
H	1.666689	1.263358	1.545137
H	2.735405	0.059104	0.949142
H	1.870932	-0.463143	-1.510924
O	3.118259	-1.135042	-1.427017
H	3.194883	-1.935981	-1.936525
O	3.713859	-1.107833	0.878462
H	3.545706	-1.224524	-0.235447
H	4.642368	-1.034214	1.077744
H	3.460843	2.296543	0.511479
H	2.012441	2.551247	-0.492286
H	3.199630	1.302910	-0.937434
C	-4.040389	0.606390	-0.379354
C	-4.160522	-0.758546	-0.167542
H	-2.677856	2.272254	-0.395267
H	-4.908272	1.194561	-0.632372
H	-5.126781	-1.231696	-0.252434
H	-3.160063	-2.580206	0.343951

TS-O3-5

C	-0.831036	0.173883	0.014679
C	0.386254	1.073833	-0.188715
C	1.698006	0.439927	-0.023525
C	1.809052	-0.930766	-0.273719
C	0.623411	-1.699734	-0.629515
C	-0.605059	-1.198455	-0.555939
O	-1.068013	0.131242	1.351023
C	3.065827	-1.515424	-0.206240
N	-1.995416	0.825724	-0.701870
O	0.244858	2.239542	-0.475775
C	2.813021	1.205067	0.272454
H	0.770563	-2.726406	-0.931468
H	-1.479335	-1.800541	-0.750559
C	-2.714206	1.830688	0.102501
H	-1.638937	1.268063	-1.540992
H	-2.731226	0.077736	-0.960076
H	-1.856418	-0.543790	1.494367
O	-3.008820	-1.371541	1.324070
H	-3.575090	-1.514772	2.075875
O	-3.901531	-0.866278	-0.820231
H	-3.602371	-1.199438	0.223404
H	-4.153798	-1.596063	-1.376763
H	-3.464954	2.283174	-0.535282
H	-2.019318	2.572175	0.471192
H	-3.195837	1.315798	0.922824
C	4.054571	0.604130	0.362289
C	4.175835	-0.755844	0.120418
H	2.686970	2.264247	0.435116
H	4.924514	1.190066	0.613393
H	5.144747	-1.227328	0.180563
H	3.172399	-2.570541	-0.409329

TS-O3-6

C	-0.907305	0.695735	-0.415610
C	-0.073625	1.915077	-0.669456
C	1.253323	1.907818	-0.624906
C	2.014554	0.721538	-0.262760
C	1.350899	-0.447972	0.118802
C	-0.116224	-0.458277	0.217316
O	-1.462440	0.300302	-1.572883
C	3.403309	0.718796	-0.293675
N	-2.006762	1.051583	0.559973
H	-0.612570	2.787764	-1.013570
H	1.813267	2.789151	-0.903124
C	2.064819	-1.585082	0.464630
O	-0.723208	-1.366065	0.737185
H	-2.495966	1.818847	0.113561
C	-1.577543	1.431580	1.904520
H	-2.812311	0.179454	0.615298
H	-2.089508	-0.727412	-1.529310
O	-2.809272	-1.667290	-1.408815
H	-2.290995	-2.457726	-1.276883
O	-3.696392	-0.783769	0.608853
H	-3.340403	-1.328613	-0.356467
H	-4.608812	-0.520721	0.516230
H	-2.430710	1.804977	2.460503
H	-1.198319	0.549094	2.406845
H	-0.804574	2.194991	1.866722
C	3.445395	-1.577649	0.419870
C	4.111309	-0.421107	0.041042
H	1.514085	-2.462969	0.765331
H	4.002441	-2.463969	0.679765
H	5.189999	-0.408125	0.007364
H	3.928741	1.616001	-0.585433

TS-O3-7

C	-0.957663	0.686395	-0.497130
C	-0.136471	1.909736	-0.806345
C	1.183638	1.936757	-0.648078
C	1.933278	0.755562	-0.230164
C	1.305207	-0.494923	-0.243209
C	-0.105056	-0.585490	-0.682716
O	-2.119500	0.687327	-1.119441
C	3.273472	0.822870	0.127599
N	-1.187506	0.696602	1.045310
H	-0.696316	2.765108	-1.152611
H	1.743767	2.838913	-0.848437
C	2.004037	-1.643279	0.089144
O	-0.575555	-1.594662	-1.134231
C	-1.991648	1.843680	1.465624
H	-0.293672	0.692819	1.524098
H	-1.758624	-0.248022	1.319398
H	-2.782291	-0.313488	-0.985559
O	-3.430356	-1.273808	-0.717950
H	-3.086981	-1.980799	-1.261094
O	-2.501281	-1.397964	1.465225
H	-3.044170	-1.440145	0.403522
H	-3.116386	-1.491213	2.187026
H	-2.297431	1.706051	2.497369
H	-1.427556	2.765716	1.370166
H	-2.864191	1.879868	0.823347
C	3.330831	-1.558186	0.469581
C	3.961799	-0.323579	0.485229
H	1.487826	-2.590012	0.045095
H	3.874170	-2.448029	0.745935
H	5.000605	-0.254674	0.769591
H	3.778778	1.777286	0.118952

TS-O4-2

C	-0.958665	-1.216844	-0.713088
C	-1.039297	0.032808	-1.216441
C	-0.077283	1.099539	-0.877320
C	1.262471	0.620527	-0.410852
C	1.446411	-0.710885	-0.060874
C	0.334281	-1.695431	-0.147371
O	-1.963530	-2.034602	-0.662145
C	2.326022	1.506068	-0.310539
H	-1.972299	0.326958	-1.671433
H	0.059110	1.801853	-1.701380
C	2.686545	-1.143594	0.387831
O	0.484100	-2.828949	0.236996
H	-2.813149	-1.402725	-0.334835
N	-0.697478	1.914511	0.239883
H	-0.001719	2.537305	0.632683
H	-1.069225	1.233582	1.017838
O	-3.544642	-0.454790	0.218675
H	-4.399737	-0.763689	0.503922
H	-2.757992	0.026497	1.194114
O	-2.010895	0.466984	1.857618
H	-1.690969	-0.216082	2.441340
C	-1.896075	2.664556	-0.164557
H	-2.196957	3.305186	0.655894
H	-2.689817	1.949107	-0.356831
H	-1.689386	3.257927	-1.049730
C	3.739791	-0.257020	0.490809
C	3.560250	1.072170	0.138850
H	2.793475	-2.184829	0.649632
H	4.702507	-0.598187	0.838186
H	4.383497	1.766697	0.203667
H	2.198041	2.538297	-0.610089

TS-O4-1

C	-1.013433	-1.345242	-0.397814
C	-1.095112	-0.129566	-0.989780
C	-0.119934	0.949671	-0.738089
C	1.264471	0.475924	-0.423171
C	1.439737	-0.815972	0.065222
C	0.293852	-1.761784	0.196502
O	-1.992730	-2.175335	-0.306149
C	2.370822	1.294807	-0.593116
H	-2.026181	0.153516	-1.455019
H	-0.093694	1.670549	-1.554192
C	2.707821	-1.261606	0.406924
O	0.438133	-2.826370	0.743805
H	-2.952114	-1.539162	-0.229855
N	-0.671754	1.730437	0.446074
H	-0.500039	1.160702	1.268493
H	-1.772420	1.740266	0.371841
O	-3.867207	-0.708701	-0.065404
H	-4.555848	-1.078439	0.479941
H	-3.550320	0.517567	0.245846
O	-3.214162	1.556907	0.456525
H	-3.844562	2.163734	0.079033
C	-0.148616	3.080021	0.656844
H	-0.678158	3.536420	1.485949
H	-0.322395	3.665397	-0.239808
H	0.913474	3.049566	0.872209
C	3.803676	-0.434710	0.250967
C	3.636424	0.842500	-0.259497
H	2.805461	-2.268669	0.781818
H	4.789316	-0.787788	0.511398
H	4.491659	1.483704	-0.407429
H	2.247579	2.283316	-1.012925

TS-O4-3

C	-0.932988	-1.328834	-0.624187
C	-1.072122	-0.057398	-1.065840
C	-0.087939	1.019756	-0.845121
C	1.250865	0.573008	-0.343141
C	1.481108	-0.759739	-0.033644
C	0.413025	-1.787520	-0.167582
O	-1.889927	-2.189562	-0.563781
C	2.280859	1.494004	-0.199641
H	-2.037534	0.235185	-1.453493
H	0.067956	1.612030	-1.750293
C	2.731501	-1.158236	0.421698
O	0.638446	-2.941020	0.100834
H	-2.814534	-1.632957	-0.130291
N	-0.687533	1.993029	0.153584
H	0.054188	2.416270	0.698140
H	-1.384617	1.446869	0.845279
O	-3.600805	-0.914675	0.478613
H	-4.472751	-0.833957	0.106882
H	-3.060883	0.107116	1.046910
O	-2.511445	0.945692	1.538593
H	-2.432881	0.729763	2.464200
C	-1.508643	3.033925	-0.469474
H	-1.962794	3.639945	0.305674
H	-2.298144	2.553340	-1.035832
H	-0.907365	3.650944	-1.129938
C	3.746861	-0.236842	0.574656
C	3.521780	1.095737	0.261279
H	2.873447	-2.203164	0.649915
H	4.715225	-0.551856	0.930988
H	4.315515	1.819485	0.364056
H	2.121913	2.529133	-0.475374

TS-O4-4

C	1.496137	-0.323259	1.140905
C	0.867219	0.773779	1.628683
C	-0.398177	1.273111	1.036780
C	-1.306674	0.200219	0.521705
C	-0.752637	-1.000517	0.097816
C	0.703778	-1.237540	0.236538
O	2.724278	-0.633787	1.326656
C	-2.678304	0.380386	0.440077
H	1.426618	1.446427	2.263418
H	-0.952756	1.908204	1.729339
C	-1.561035	-2.000590	-0.421198
O	1.236385	-2.153841	-0.348085
H	3.212249	-0.521561	0.103156
N	0.018786	2.160438	-0.114609
H	0.686382	2.816950	0.272096
H	0.686113	1.524086	-0.893007
O	3.395408	-0.334892	-0.969178
H	3.361723	-1.205949	-1.364359
H	2.462812	0.295801	-1.360205
O	1.482762	0.923534	-1.700542
H	1.062062	0.509067	-2.450004
C	-1.043692	2.896325	-0.793887
H	-1.639779	3.466887	-0.084974
H	-1.687710	2.197122	-1.314638
H	-0.599136	3.572214	-1.516734
C	-2.927739	-1.813357	-0.503869
C	-3.487494	-0.623525	-0.065846
H	-1.094370	-2.920045	-0.739279
H	-3.559125	-2.595377	-0.896193
H	-4.556014	-0.479224	-0.111252
H	-3.119531	1.304030	0.787858

TS-O4-5

C	-1.466748	-0.491334	-1.101328
C	-0.919295	0.634253	-1.616961
C	0.327047	1.223078	-1.065754
C	1.301530	0.221468	-0.528735
C	0.823825	-0.993006	-0.054875
C	-0.617469	-1.326629	-0.174738
O	-2.677008	-0.886350	-1.269796
C	2.661257	0.485154	-0.472991
H	-1.524302	1.251427	-2.266478
H	0.834899	1.859559	-1.792382
C	1.696108	-1.922582	0.491687
O	-1.090077	-2.251675	0.439718
H	-3.192470	-0.659698	-0.117674
N	-0.117404	2.129963	0.058491
H	-0.816758	2.742018	-0.344422
H	-0.754758	1.490596	0.876138
O	-3.446527	-0.270754	0.911843
H	-4.253419	0.236669	0.889026
H	-2.497444	0.350888	1.333551
O	-1.524830	0.915451	1.708365
H	-1.090089	0.376233	2.365857
C	0.917290	2.939644	0.695479
H	1.481048	3.506997	-0.042170
H	1.596716	2.292402	1.237657
H	0.449214	3.623483	1.395621
C	3.049804	-1.651292	0.550714
C	3.533870	-0.448614	0.059976
H	1.287886	-2.855266	0.849402
H	3.730449	-2.378655	0.965246
H	4.592390	-0.240098	0.086180
H	3.042691	1.419474	-0.860866

APPENDIX B

SAMPLE GAUSSIAN INPUT FILES

This appendix includes different sample input files that were used in the calculations of energies of the energy minima and transition states.

A sample input file for calculation in gas-phase using Cartesian coordinates system

```
# mPWB95/6-31+G(d,p)
IOp(3/76=0560004400)
SCF=(Conver=9,MaxCycle=200) Integral=(grid=ultrafine)
OPT=(Verytight,Calcall,Maxcycle=20)

Hydronaphtoquinone - Optimization - 1,4 - Cis

0 1
C1 -0.716573   -0.158013    0.000000
C2 0.452561   -0.833013    0.000000
C3 0.452561   -2.183013    0.000000
C4 -0.716573   -2.858013    0.000000
C5 -1.885707   -2.183013    0.000000
C6 -1.885707   -0.833013    0.000000
H7 1.396529   -2.728013    0.000000
H8 -0.716573   -3.948013    0.000000
H9 -2.829675   -2.728013    0.000000
H10 -2.829675   -0.288013    0.000000
C11 -0.716573    1.191987    0.000000
C12 0.452561    1.866987    0.000000
C13 1.621695    1.191987    0.000000
C14 1.621695   -0.158013    0.000000
H15 2.565663    1.736987    0.000000
O16 -1.755804    1.791987    0.000000
O17 0.452561    3.266987    0.000000
O18 2.660926   -0.758013    0.000000
H19 -0.527375    3.278147    0.000000
```

A sample input file for transition state calculation in gas phase using Cartesian coordinates system

```
# mPWB95/6-31+G(d,p)
IOp(3/76=0560004400)
SCF=(Conver=9,MaxCycle=200) Integral=(grid=ultrafine)
OPT=(TS,Noeigentest,Verytight,Calcall,Maxcycle=20)

Transition State of 1,4 addition at C1 - Conformation 1

0 1
C1   -0.174259    1.178805   -0.506494
C2    0.867439    0.387374   -0.775298
C3    0.783864   -1.092977   -0.646988
C4   -0.497363   -1.628363   -0.028814
C5   -1.664348   -0.759861   -0.033711
C6   -1.485319    0.617472   -0.219538
O7   -0.101397    2.523775   -0.533942
O8   -0.479382   -2.744667    0.446368
H9    0.761453    2.799668   -0.099252
N10   1.909566   -1.592913    0.163821
H11   1.592399   -2.426413    0.650061
H12   2.203841   -0.745775    0.926648
O13   2.288433    2.502913    0.806865
H14   3.004758    3.105916    0.980231
H15   2.439158    1.538725    1.312423
O16   2.531763    0.279099    1.640158
H17   2.443544    0.169196    2.583243
C18   3.102504   -1.890531   -0.636243
H19   3.900745   -2.195468    0.031792
H20   3.392782   -0.991365   -1.161395
H21   2.893888   -2.689317   -1.343524
H22   0.850011   -1.552628   -1.639670
O23   2.082637    0.817286   -1.156483
H24   2.329691    1.599293   -0.616936
C25  -2.594795    1.448908   -0.112814
C26  -3.841770    0.914435    0.147926
C27  -4.013729   -0.452308    0.331799
C28  -2.917299   -1.284423    0.257525
H29  -2.456583    2.510340   -0.235100
H30  -4.694414    1.573097    0.216217
H31  -4.992035   -0.855671    0.539433
H32  -3.002185   -2.347639    0.421244
```

A sample input file for a transition state calculation in gas phase using mixed coordinates system

```
# mPWB95/6-31+G(d,p)
IOp(3/76=0560004400)
SCF=(Conver=9,MaxCycle=200) Integral=(grid=ultrafine)
OPT=(TS,Noeigentest,Verytight,Calcall,Maxcycle=20)

Transition State of 1,2 addition at C1 - Conformation 1

0 1
C1   0.200879    0.609772   -0.122980
C2  -1.024813    1.470280   -0.078321
C3  -2.256907    0.982404   -0.013730
C4  -2.507408   -0.468761   -0.004532
C5  -1.338197   -1.344434   -0.175651
C6  -0.103969   -0.859045   -0.235464
O7   1.052479    1.065565   -1.048938
O8  -3.626434   -0.915728    0.119426
N9   0.882856    0.775568    1.255075
H10 -1.545594   -2.399070   -0.272556
O11  C6 1.43  C1 120. C2 180.
H12  1.205681    1.734680    1.313253
C13  N9 1.47 C1 109.5 O7 180.
H14  1.773786    0.114748    1.322831
H15  1.896874    0.346981   -1.214749
O16  2.823670   -0.548114   -1.195887
O17  2.986069   -0.638027    1.183250
H18  3.062992   -0.664224    0.082461
H19  3.111751   -1.506375    1.554913
H20  3.568561   -0.355385   -1.757454
C21 C2 1.35 C1 120. C6 180.
C22 C21 1.35 C2 120. C1 180.
C23 C22 1.35 C21 120. C2 0.
C24 C23 1.35 C22 120. C21 0.
H25 C21 1.09 C2 120. C1 0.
H26 C22 1.09 C21 120. H25 0.
H27 C23 1.09 C22 120. H26 0.
H28 C24 1.09 C3 120. C4 0.
H29 O11 0.98 C6 110. C1 -45.
H30 C13 1.09 N9 109.5 C1 180.
H31 C13 1.09 N9 109.5 C1 60.
H32 C13 1.09 N9 109.5 C1 -60.
```